U.S. DEPARTMENT OF COMMERCE
National Technical Information Service

PB-280 203

Identification of Components of Energy-Related Wastes and Effluents

Research Triangle Inst, Research Triangle Park, N C

Prepared for

Environmental Research Lab, Athens, Ga

Jan 78

EPA

PB 280 203

United States
Environmental Protection
Agency

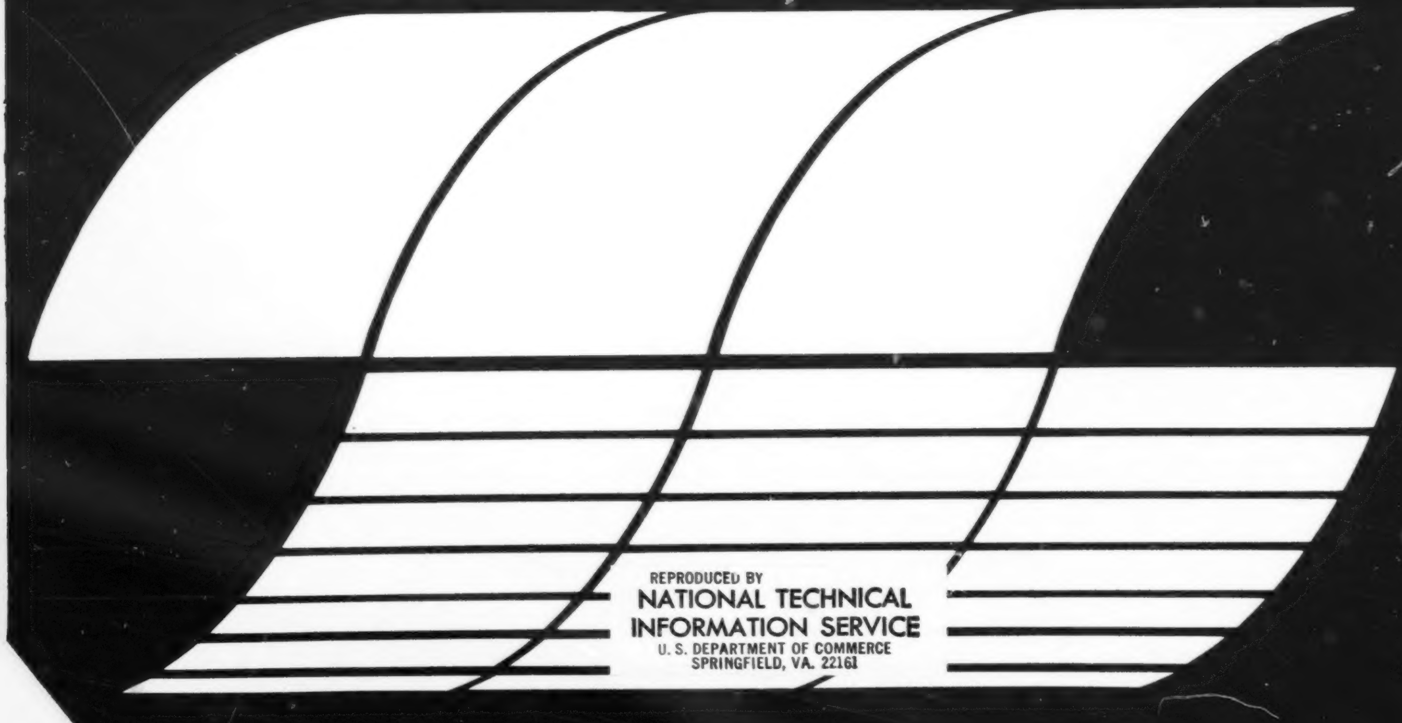
Office of
Research and
Development

Environmental Research
Laboratory
Athens, Georgia 30605

EPA-600/7-78-004
January 1978

IDENTIFICATION OF COMPONENTS OF ENERGY-RELATED WASTES AND EFFLUENTS

Interagency Energy-Environment Research and Development Program Report



REPRODUCED BY
NATIONAL TECHNICAL
INFORMATION SERVICE
U. S. DEPARTMENT OF COMMERCE
SPRINGFIELD, VA. 22161

RESEARCH REPORTING SERIES

Research reports of the Office of Research and Development, U.S. Environmental Protection Agency, have been grouped into nine series. These nine broad categories were established to facilitate further development and application of environmental technology. Elimination of traditional grouping was consciously planned to foster technology transfer and a maximum interface in related fields. The nine series are:

1. Environmental Health Effects Research
2. Environmental Protection Technology
3. Ecological Research
4. Environmental Monitoring
5. Socioeconomic Environmental Studies
6. Scientific and Technical Assessment Reports (STAR)
7. Interagency Energy-Environment Research and Development
8. "Special" Reports
9. Miscellaneous Reports

This report has been assigned to the INTERAGENCY ENERGY-ENVIRONMENT RESEARCH AND DEVELOPMENT series. Reports in this series result from the effort funded under the 17-agency Federal Energy/Environment Research and Development Program. These studies relate to EPA's mission to protect the public health and welfare from adverse effects of pollutants associated with energy systems. The goal of the Program is to assure the rapid development of domestic energy supplies in an environmentally-compatible manner by providing the necessary environmental data and control technology. Investigations include analyses of the transport of energy-related pollutants and their health and ecological effects; assessments of, and development of, control technologies for energy systems; and integrated assessments of a wide range of energy-related environmental issues.

This document is available to the public through the National Technical Information Service, Springfield, Virginia 22161.

TECHNICAL REPORT DATA

(Please read Instructions on the reverse before completing)

1. REPORT NO. EPA-600/7-78-004	2.	3. RECIPIENT'S ACCESSION NO. PB280203
4. TITLE AND SUBTITLE IDENTIFICATION OF COMPONENTS OF ENERGY-RELATED WASTES AND EFFLUENTS		5. REPORT DATE January 1978 issuing date
		6. PERFORMING ORGANIZATION CODE
7. AUTHOR(S) E. D. Pellizzari		8. PERFORMING ORGANIZATION REPORT NO.
9. PERFORMING ORGANIZATION NAME AND ADDRESS Research Triangle Institute P. O. Box 12194 Research Triangle Park, NC 27709		10. PROGRAM ELEMENT NO. 1NE625
		11. CONTRACT/GRANT NO. 68-03-2368
12. SPONSORING AGENCY NAME AND ADDRESS Environmental Research Laboratory - Athens, GA Office of Research and Development U. S. Environmental Protection Agency Athens, GA 30605		13. TYPE OF REPORT AND PERIOD COVERED Final
		14. SPONSORING AGENCY CODE EPA/600/01
15. SUPPLEMENTARY NOTES		

16. ABSTRACT

A state-of-the-art review on the characterization of organic and elemental substances in energy-related liquid and solid effluents was conducted. Previous and ongoing research programs and reports were reviewed to summarize the existing and probable future data on chemical elements and organic compounds in solid waste and aqueous effluents from (a) coal liquefaction and gasification plants, (b) coal-fired power plants, (c) oil-shale processors, (d) oil refineries, (e) coal mines and (f) geothermal energy. The reliability of existing information and the probability of accumulation of adequate data from current and past contracts and projects was evaluated according to preselected criteria.

Based upon the absence of adequate data on the composition of energy samples, a chemical characterization program was conducted for several energy-related processes. The necessary preconcentrations and purification were performed on these samples and the volatile and semi-volatile organic compounds were identified and quantified. Samples for organic and mercury analysis were subjected to a single analytical protocol in each case to permit comparison among samples. Organic constituents were analyzed by gas chromatography/mass spectrometry/computer and elemental components were determined and measured by spark-source mass spectrometry for all the elements in the periodic chart through uranium except oxygen, helium, hydrogen, neon, krypton, xenon, radon, nitrogen and carbon. The analysis of mercury was performed by flameless atomic absorption spectrophotometry.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group
Energy	Organic chemicals	48A
Elements	Solid wastes	68D
Effluents	Coal liquefaction	97F
Coal gasification	Coal-fired power plants	97G
Refineries	Oil-shale processing	
	Geothermal energy	

18. DISTRIBUTION STATEMENT RELEASE TO PUBLIC	19. SECURITY CLASS *(This Report)* UNCLASSIFIED	21. NO. OF PAGES 525
	20. SECURITY CLASS *(This page)* UNCLASSIFIED	22. PRICE A22-A01

EPA Form 2220-1 (9-73)

☆ U.S. GOVERNMENT PRINTING OFFICE: 1978— 757-140/6673

EPA-600/7-78-004
January 1978

IDENTIFICATION OF COMPONENTS OF ENERGY-RELATED WASTES AND EFFLUENTS

by

Edo D. Pellizzari
Research Triangle Institute
Research Triangle Park, North Carolina 27709

Contract No. 68-03-2368

Project Officer

Ann Alford
Analytical Chemistry Branch
Environmental Research Laboratory
Athens, Georgia 30605

ENVIRONMENTAL RESEARCH LABORATORY
OFFICE OF RESEARCH AND DEVELOPMENT
U.S. ENVIRONMENTAL PROTECTION AGENCY
ATHENS, GEORGIA 30605

DISCLAIMER

This report has been reviewed by the Environmental Research Laboratory, U.S. Environmental Protection Agency, Athens, Georgia, and approved for publication. Approval does not signify that the contents necessarily reflect the views and policies of the U.S. Environmental Protection Agency, nor does mention of trade names or commercial products constitute endorsement or recommendation for use.

FOREWORD

Nearly every phase of environmental protection depends on a capability to identify and measure specific pollutants in the environment. As part of this Laboratory's research on the occurrence, movement, transformation, impact, and control of environmental contaminants, the Analytical Chemistry Branch develops and assesses techniques for identifying and measuring chemical constituents of water and soil.

Efforts to achieve our national goal of energy independence will require increasing utilization of our country's vast domestic coal reserves as well as resources available from oil shale and tar sands. Production of synthetic fuels using coal gasification, coal liquefaction, oil-shale retorting, and other processes offers promise of meeting many of our energy needs. Of collateral importance with the production of energy, however, is assuring that toxic or undesirable substances in energy process effluent are identified and properly controlled to prevent human health problems and reduce environmental degradation. This report provides a state-of-the-art review of existing and probable future data on organic compounds and chemical elements in solid waste and aqueous effluents from several synthetic fuel processes so that potential environmental pollution problems can be anticipated.

David W. Duttweiler
Director
Environmental Research Laboratory
Athens, Georgia

ABSTRACT

A state-of-the-art review on the characterization of organic and elemental substances in energy-related liquid and solid effluents was conducted. Previous and on-going research programs and reports were reviewed to summarize the existing and probable future data on chemical elements and organic compounds in solid waste and aqueous effluents from (a) coal liquefaction and gasification plants, (b) coal-fired power plants, (c) oil-shale processors, (d) oil refineries, (e) coal mines and (f) geothermal energy. The reliability of existing information and the probability of accumulation of adequate data from current and past contracts and projects was evaluated according to preselected criteria.

Based upon the absence of adequate data on the composition of energy samples, a chemical characterization program was conducted for several energy-related processes. The necessary preconcentrations and purifications were performed on these samples and the volatile and semi-volatile organic compounds were identified and quantified. Samples for organic and mercury analysis were subjected to a single analytical protocol in each case to permit comparison among samples. Organic constituents were analyzed by gas chromatography/mass spectrometry/computer and elemental components were determined and measured by spark-source mass spectrometry for all the elements in the periodic chart through uranium except oxygen, helium, hydrogen, neon, krypton, xenon, radon, nitrogen and carbon. The analysis of mercury was performed by flameless atomic absorption spectrophotometry.

CONTENTS

Abstract iv
Figures vii
Tables xiii
Acknowledgments. xxiv

1. Introduction 1
2. Conclusions. 6
3. Recommendations. 8
4. Program Objectives 9
5. State-of-the-Art Review on Characterization of Organic and Elemental Substances in Energy-Related Effluents. 10
6. Samples and Sampling Procedure 29
7. Physical Methods of Analysis 35
8. Results and Discussion 59

References 90

Appendices

A. Abstracts of Technical Reports and Current Projects on Characterization and Assessment of Effluents from Energy-Related Processes. 94
   Section I - Oil-Shale Processing 95
      Part I: Technical Reports. 95
      Part II: Current Projects. 106
   Section II - Coal Gasification and Liquefaction. 109
      Part I: Technical Reports. 109
      Part II: Current Projects. 175
   Section III - Coal-Fired Power Plants. 188
      Part I: Technical Reports. 188
      Part II: Current Projects. 208

CONTENTS (cont'd)

Section IV - Coal Related Pollution. 212
  Part I: Technical Reports. 212
  Part II: Current Projects. 220
Section V - Oil Refineries 227
  Part I: Technical Reports. 227
  Part II: Current Projects. 231
Section VI - Tar Sands 232
  Part I: Technical Reports. 232
  Part II: Current Projects. 233
B. Elemental Constituents in Liquid and Solid Effluents From Energy-Related Processes 236
  Part I: Samples from *In Situ* Oil-Shale Gasification 237
  Part II: Samples from Low Btu Gasification of Rosebud Coal. . 240
  Part III: Samples from *In Situ* Coal Gasification in Gillette, WY. 247
  Part IV: Samples from *In Situ* Coal Gasification in Hanna, WY. 265
C. Volatile Organic Substances in Liquid and Solid Effluents From Energy-Related Processes. 285
  Part I: Samples from Oil-Shale Processing 286
  Part II: Samples from Low Btu Gasification of Rosebud Coal. . 295
  Part III: Samples from *In Situ* Coal Gasification in Gillette, WY. 311
  Part IV: Samples from *In Situ* Coal Gasification in Hanna, WY. 354
D. Semi-Volatile Organic Substances in Liquid and Solid Effluents from Energy-Related Processes. 401
  Part I: Samples from Oil-Shale Processing 402
  Part II: Samples from Low Btu Gasification of Rosebud Coal. . 412
  Part III: Samples from *In Situ* Coal Gasification in Gillette, WY. 426
  Part IV: Samples from *In Situ* Coal Gasification in Hanna, WY. 459

FIGURES

Number | | Page
1 Calibration curve for total mercury analysis in aqueous samples. 39
2 Apparatus for VOA purge 44
3 Schematic for recovery and analysis of semi-volatile organics from water or liquid tar samples 46
4 Thermal desorption inlet-manifold 48
5 Schematic diagram of gc-ms computer system and library search system. 50
6 Mass fragmentogram (m/e 236, 186, 71, 114, 67) of volatile organics in product water (-13L) from in situ coal gasification (LERC, ERDA). 65
7 Mass fragmentogram (m/e 186, 106, 107) of volatile organics in product water (-13L) from in situ coal gasification (LERC, ERDA) 66
8 Mass fragmentograms (m/e 186, 121, 94, 95, 120) of volatile organics in product water (-13L) from in situ coal gasification (LERC, ERDA). 67
9 Mass fragmentograms (m/e 186, 85) for volatile organics in product water (-13L) from in situ coal gasification (LERC, ERDA) 68
10 Mass fragmentograms (m/e 186, 105) of volatile organics in product water (-13L) from in situ coal gasification (LERC, ERDA) 69
11 Mass fragmentograms (m/e 186, 131) of volatile organics in product water (-13L) from in situ coal gasification (LERC, ERDA) 70
12 Mass fragmentograms (m/e 186, 156, 152) of volatile organics in product water (-13L) from in situ coal gasification (LERC, ERDA) 71

FIGURES (cont'd)

Number		Page
13	Total ion current chromatogram obtained by gc-ms of semi-volatile organics in acid fraction of product water (-8L) *in situ* coal gasification (LERC, ERDA).	73
14	Gas-liquid chromatogram (flame detection) of acid fraction from product water (-8L) obtained during *in situ* coal gasification	74
15	On-the-fly FT-IR spectrum of peak No. 6 (ca. 60 ng) in Fig. 14	75
16	On-the-fly FT-IR spectrum of peak No. 8 (ca. 125 ng) in Fig. 14	75
17	On-the-fly FT-IR spectrum of peak No. 10 (ca. 175 ng) in Fig. 14	76
18	On-the-fly FT-IR spectrum of peak No. 12 (ca. 180 ng) in Fig. 14	76
19	On-the-fly FT-IR spectrum of peak No. 14 (ca. 110 ng) in Fig. 14	78
20	On-the-fly FT-IR spectrum of peak No. 21 (>3 μg) in Fig. 14.	78
21	On-the-fly FT-IR spectrum of peak No. 22 (ca. 80 ng) in Fig. 14	79
22	On-the-fly FT-IR spectrum of peak No. 23 (ca. 75 ng) in Fig. 14	79
23	On-the-fly FT-IR spectrum of peak No. 18 (ca. 30 ng) in Fig. 14	80
24	"Chemigram" (IR detection of acid fraction from product water obtained during *in situ* coal gasification . . .	84
25	On-the-fly FT-IR spectrum of methyl hexanoate (Files 20-30 of chemigram co-added and smoothed).	85
26	On-the-fly FT-IR spectrum of methyl heptanoate (Files 31-35 of chemigram co-added and smoothed).	86
27	On-the-fly FT-IR spectrum of methyl octanoate (Files 41-47 of chemigram co-added)	87

FIGURES (cont'd)

Number — Page

28 On-the-fly FT-IR spectrum of methyl nonanoate (Files 52-57 of chemigram co-added). 88

29 On-the-fly FT-IR spectrum of phenol (File 197 of chemigram). 89

C1 Profile of volatile organics in aqueous sample from 150 Ton oil-shale retort (LERC, ERDA). 286

C2 Profile of volatile organics in aqueous condensate (-1L) from low btu gasification of Rosebud coal (MERC, ERDA) 292

C3 Profile of volatile organics in aqueous condensate (-2L) from low btu gasification of coal (MERC, ERDA) 295

C4 Profile of volatile organics in aqueous sample (-1L) from dewatering well #5 (LLL, ERDA) 308

C5 Profile of volatile organics in blended liquid sample (-2L) from dewatering wells #1 and 6 (LLL, ERDA) 311

C6 Profile of volatile organics in process water (-3L) from *in situ* coal gasification (LLL, ERDA). 314

C7 Profile of volatile organics in product tar (-4T) from *in situ* coal gasification (LLL, ERDA) 317

C8 Profile of volatile organics in liquid process composite (-6L) from *in situ* coal gasification (LLL, ERDA) . . . 322

C9 Profile of volatile organics in water sample (-8L) from environmental well #4 (LLL, ERDA). 327

C10 Profile of volatile organics in water sample (-9L) from environmental well #5 (LLL, ERDA). 330

C11 Profile of volatile organics in water sample (-11L) from dewatering well #5 (LLL, ERDA) 335

C12 Profile of volatile organics in water sample (-14L) from environmental monitoring well #2, post-gasification (LLL, ERDA). 340

C13 Profile of volatile organics in water sample (-17L) from dewatering well #5, post-gasification (LLL, ERDA). . . 346

C14 Profile of volatile organics in liquid sample (-19L) from production well #1, post-gasification (LLL, ERDA). . . 351

FIGURES (cont'd)

Number		Page
C15	Profile of volatile organics in product water sample (-14L) in situ coal gasification (LERC, ERDA)	372
C16	Profile of volatile organics in product water sample (-16L) during well 7-8 in situ coal gasification (LERC, ERDA)	378
C17	Profile of volatile organics in product water (-18L) during well 7-8 in situ coal gasification (LERC, ERDA). . . .	384
C18	Profile of volatile organics in product water (-19L) from in situ coal gasification (LERC, ERDA)	387
C19	Profile of volatile organics in ground water sample from corehole #3 (-20L) after in situ coal gasification (LERC, ERDA)	390
C20	Profile of volatile organics in post-gasification water sample (-22L) from well #8, Hanna 1 (LERC, ERDA) . . .	392
C21	Profile of volatile organics in post-gasification water sample (-23L) from well WQ-1 after in situ coal gasification (LERC, ERDA).	395
C22	Profile of volatile organics in post-gasification water sample (-25L) from well #4, Hanna 11 (LERC, ERDA). . .	399
D1	Profile of semi-volatile acid fraction from aqueous boiler blow-down sample obtained during in situ oil-shale processing	403
D2	Profile of semi-volatile basic fraction from aqueous boiler blow-down sample obtained from in situ oil-shale processing	404
D3	Profile of semi-volatile organics in neutral fraction of Omega-9 retort water (after incubation) from in situ oil-shale processing (LERC, ERDA).	409
D4	Profile of semi-volatile organics in acidic fraction of Omega-9 retort water (after incubation) from in situ oil-shale processing (LERC, ERDA).	410
D5	Profile of semi-volatile organics in basic fraction of Omega-9 retort water (after incubation) from in situ oil-shale processing (LERC, ERDA).	411

FIGURES (cont'd)

Number		Page
D6	Profile of semi-volatile organics in neutral fraction of tar condensate (-7T) from low btu Rosebud coal gasification (MERC, ERDA).	424
D7	Profile of semi-volatile organics in basic fraction of tar-condensate (-7T) from low btu gasification of Rosebud coal (MERC, ERDA).	425
D8	Profile of semi-volatile organics in neutral fraction of process tar (-4L) from *in situ* coal gasification (LLL, ERDA).	431
D9	Profile of semi-volatile organics in acid fraction of process tar (-4L) from *in situ* coal gasification (LLL, ERDA) .	432
D10	Profile of semi-volatile organics in neutral fraction of water sample (-10L) from dewatering well #4 (LLL, ERDA).	445
D11	Profile of semi-volatile organics in acid fraction of water sample (-10L) from dewatering well #4 (LLL, ERDA). . .	446
D12	Profile of semi-volatile organics in basic fraction of water sample (-10L) from dewatering well #4 (LLL, ERDA).	447
D13	Profile of semi-volatile organics in neutral fraction from post-gasification water sample (-21L) obtained from well #1, Hanna 1 (LERC, ERDA).	489
D14	Profile of semi-volatiles in acid fraction of post-gasification water sample (-21L) from *in situ* coal gasification (LERC, ERDA).	490
D15	Profile of semi-volatile organics in basic fraction from post-gasification water sample (-21L) obtained from well #1, Hanna 1 (LERC, ERDA).	491
D16	Profile of semi-volatile organics in neutral fraction from post-gasification water sample (-24L) obtained from well #4, Hanna 1 (LERC, ERDA)	495

FIGURES (cont'd)

Number		Page
D17	Profile of semi-volatile organics in acid fraction from post-gasification water sample (-24L) obtained from well #1, Hanna 1 (LERC, ERDA)	496
D18	Profile of semi-volatile organics in basic fraction from post-gasification water sample (-24L) obtained from well #1, Hanna 1 (LERC, ERDA)	497

TABLES

Number		Page
1	Organic Compounds Identified in Effluents from Energy-Related Processes.	12
2	Elemental Compounds Identified in Effluents from Energy-Related Processes	21
3	Description of Energy-Related Liquid and Solid Effluents Received and Characterized for Elemental and Organic Substances	32
4	Instrumental Operating Parameters for Flameless Atomic Absorption Spectrophotometer	37
5	Operating Parameters for GLC-MS-COMP System	51
6	Percent Recovery of Selected Radiolabeled Compounds Using Liquid/Liquid Extraction Method.	61
7	Examples of Relative Molar Response (RMR) Factors for Several Compounds Based Upon Total Ion Current Monitor.	62
8	Examples of Relative Molar Response Factors for Several Compounds Based Upon Selected Fragment Ions.	63
9	Semi-Volatile Organic Acids in Product Water (-8L) From In Situ Coal Gasification (LERC, ERDA)	81
B1	Elemental Concentrations in Liquid Sample From 150 Ton Oil-Shale Retort Processing Experiment (LERC).	237
B2	Elemental Concentrations in Discarded Cavern Oil-Shale From In Situ Oil-Shale Processing (OOS).	238
B3	Elemental Concentrations in Boiler Blow-Down Water From In Situ Oil-Shale Processing (OOS)	239
B4	Elemental Concentrations in Liquid Condensate (-1L) From Rosebud Coal During Low Btu Coal Gasification (MERC) .	240
B5	Elemental Concentrations in Liquid Condensate (-2L) From Rosebud Coal During Low Btu Coal Gasification (MERC) .	241

TABLES (cont'd)

Number Page

B6 Elemental Concentrations in Liquid Condensate (-3L) From Rosebud Coal During Low Btu Coal Gasification (MERC) . . 242

B7 Elemental Concentrations in Liquid Condensate (-4L) From Rosebud Coal During Low Btu Coal Gasification (MERC) . . 243

B8 Elemental Concentrations in Liquid Condensate (-5T) From Rosebud Coal During Low Btu Coal Gasification (MERC) . . 244

B9 Elemental Concentrations in Liquid Condensate (-6T) From Rosebud Coal During Low Btu Coal Gasification (MERC) . . 245

B10 Elemental Concentrations in Liquid Condensate (-7T) From Rosebud Coal During Low Btu Coal Gasification (MERC) . . 246

B11 Elemental Concentrations in Liquid Sample (-1L) From Dewatering Well #5 Prior to *In Situ* Coal Gasification (LLL) 247

B12 Elemental Concentrations in a Blend Liquid Sample (-2L) From Dewatering Wells #1 and 6 (LLL) 248

B13 Elemental Concentrations in Process Water Sample (-3L) From *In Situ* Coal Gasification (LLL) 249

B14 Elemental Concentrations in Process Tar (-4T) From *In Situ* Coal Gasification (LLL) 250

B15 Elemental Concentrations in Well Water From Perm #5 (-5L) *In Situ* Coal Gasification Experiment (LLL) 251

B16 Elemental Concentrations in Well Water - EW4 (-8L) From *In Situ* Coal Gasification Experiment (LLL) 252

B17 Elemental Concentrations in Well Water - EW5 (-9L) From *In Situ* Coal Gasification Experiment (LLL) 253

B18 Elemental Concentrations in Well Water - DW#4 (-10L) From *In Situ* Coal Gasification Experiment (LLL) 254

B19 Elemental Concentrations in Well Water - DW#5 (-11L) From *In Situ* Coal Gasification Experiment (LLL) 255

B20 Elemental Concentrations in Water Sample From EM-1 Well (-12L) After *In Situ* Coal Gasification (LLL) 256

B21 Elemental Concentrations in Water Sample From EM-4 Well (-13L) After *In Situ* Coal Gasification 257

TABLES (cont'd)

Number Page

B22 Elemental Concentrations in Water Sample From EM-2 Well (-14L) After In Situ Coal Gasification. 258

B23 Elemental Concentrations in Tar Sample (-15T) From Production Well #1 After In Situ Coal Gasification (LLL) 259

B24 Elemental Concentrations in Water Sample (-16L) From Well DW-4 From In Situ Coal Gasification Experiment (LLL). . 260

B25 Elemental Concentrations in Water Sample (-17L) From Well DW-5 From In Situ Coal Gasification Experiment (LLL). . 261

B26 Elemental Concentrations in Water Sample (-18L) From Well DW-4 From In Situ Coal Gasification Experiment (LLL). . 262

B27 Elemental Concentrations in Water Sample (-19L) From Production Well #1 After In Situ Coal Gasification (LLL) . 263

B28 Elemental Concentrations in Water Sample (-20L) From Production Well #1 After In Situ Coal Gasification (LLL) . 264

B29 Elemental Concentrations in Seam Water From Well #6 (Hanna #2) Prior to In Situ Coal Gasification (LERC) 265

B30 Elemental Concentrations in Seam Water From Well #5 (Hanna #2) Prior to In Situ Coal Gasification (LERC) 266

B31 Elemental Concentrations in Product Water (-8L) From Well 5-6 Linkage During In Situ Coal Gasification (LERC) . . 267

B32 Elemental Concentrations in Product Water (-9L) From Well 5-6 Linkage During In Situ Coal Gasificiation (LERC). . 268

B33 Elemental Concentrations in Product Tar (-10S) From Well 5-6 Linkage During In Situ Coal Gasification (LERC) . . 269

B34 Elemental Concentrations in Product Water (-11L) From Well 5-6 Linkage During In Situ Coal Gasification (LERC) . . 270

B35 Elemental Concentrations in Product Tar (-12S) From Well 5-6 Linkage During In Situ Coal Gasification (LERC) . . 271

B36 Elemental Concentrations in Product Water (-13L) From Well 5-6 Linkage During In Situ Coal Gasification (LERC) . . 272

B37 Elemental Concentrations in Product Water (-14L) From Well 7-8 In Situ Coal Gasification (LERC). 273

TABLES (cont'd)

Number Page

B38 Elemental Concentrations in Product Tar (-15S) From Well 7-8 *In Situ* Coal Gasification (LERC). 274

B39 Elemental Concentrations in Product Water (-16L) From Well 7-8 *In Situ* Coal Gasification (LERC). 275

B40 Elemental Concentrations in Product Tar (-17S) From Well 7-8 *In Situ* Coal Gasification (LERC). 276

B41 Elemental Concentrations in Product Water (-18L) From Well 7-8 *In Situ* Coal Gasification (LERC). 277

B42 Elemental Concentrations in Product Water (-19L) From Well 7-8 *In Situ* Coal Gasification (LERC). 278

B43 Elemental Concentrations in Ground Water Sample (Core Hole #3) From *In Situ* Coal Gasification Experiment (LERC). . . . 279

B44 Elemental Concentrations in Post-Gasification Water Sample (Well #1, Hanna #1) After *In Situ* Coal Gasification Experiment (LERC) 280

B45 Elemental Concentrations in Post-Gasification Water Sample (Well #8, Hanna #1) After *In Situ* Coal Gasification Experiment (LERC) 281

B46 Elemental Concentrations in Post-Gasification Water Sample (Well-WQ-1) From *In Situ* Coal Gasification Experiment (LERC). 282

B47 Elemental Concentrations in Post-Gasification Water Sample (Well #1, Hanna #2) From *In Situ* Coal Gasification Experiment (LERC) 283

B48 Elemental Concentrations in Post-Gasification Water Sample (Well #4, Hanna #2) From *In Situ* Coal Gasification Experiment (LERC) 284

C1 Volatile Organics in Aqueous Sample From 150 Ton Oil-Shale Retort Processing (LERC, ERDA). 287

C2 Volatile Organics in Aqueous Boiler Blow-Down Sample From *In Situ* Oil-Shale Processing (OCC). 288

C3 Volatile Organics in Omega-9 Retort Water From *In Situ* Oil-Shale Processing Prior to Incubation at 75°F (LERC, ERDA) 289

TABLES (cont'd)

Number | | Page
C4 Volatile Organics in Omega-9 Retort Water From In Situ Oil-Shale Processing After Incubation at 75°F for 2 Months (LERC, ERDA). 291
C5 Volatile Organics in Aqueous Condensate (-1L) From Low Btu Gasification of Rosebud Coal (MERC, ERDA). 293
C6 Volatile Organics in Aqueous Condensate (-2L) From Low Btu Gasification of Rosebud Coal (MERC, ERDA). 296
C7 Volatile Organics in Tar (-3T) From Knock-Out Chamber During Low Btu Gasification of Rosebud Coal (MERC, ERDA). . . 298
C8 Volatile Organics in Aqueous Condensate (-4L) From Low Btu Gasification of Rosebud Coal (MERC, ERDA). 300
C9 Volatile Organics in Tar (-5T) From Knock-Out Chamber During Low Btu Gasification of Rosebud Coal (MERC, ERDA). . . 302
C10 Volatile Organics in Aqueous Condensate (-6L) From Low Btu Gasification of Rosebud Coal (MERC, ERDA). 304
C11 Volatile Organics in Tar (-7T) From Knock-Out Chamber During Low Btu Gasification of Rosebud Coal (MERC, ERDA). . . 306
C12 Volatile Organics in Aqueous Sample (-1L) From Dewatering Well #5 (LLL, ERDA). 309
C13 Volatile Organics in Blended Liquid Sample (-12L) From Dewatering Wells #1 and 6 (LLL, ERDA). 312
C14 Volatile Organics in Process Water (-3L) From In Situ Coal Gasification (LLL, ERDA) 315
C15 Volatile Organics in Product Tar (-4T) From In Situ Coal Gasification (LLL, ERDA) 318
C16 Volatile Organics in Water (-5T) From Permeation Well #5 (LLL, ERDA). 321
C17 Volatile Organics in Liquid Process Composite (-6L) From In Situ Coal Gasification (LLL, ERDA). 323
C18 Volatile Organics in Liquid Process Composite (-7L) From In Situ Coal Gasification (LLL, ERDA). 325
C19 Volatile Organics in Water Sample (-8L) From Environmental Well #4 (LLL, ERDA). 328

TABLES (cont'd)

Number Page

C20 Volatile Organics in Water Sample (-9L) From Environmental Well #5 (LLL, ERDA). 331

C21 Volatile Organics in Water (-10L) From Dewatering Well #5 (LLL, ERDA). 333

C22 Volatile Organics in Water (-11L) From Dewatering Well #5 (LLL, ERDA). 336

C23 Volatile Organics in Water (-12L) From Environmental Monitoring Well #1, Post-Gasification (LLL, ERDA). 338

C24 Volatile Organics in Water (-13L) From Environmental Monitoring Well #4, Post-Gasification (LLL, ERDA). 339

C25 Volatile Organics in Water (-14L) From Environmental Monitoring Well #2, Post-Gasification (LLL, ERDA). 341

C26 Volatile Organics in Liquid Sample (-15T) From Production Well #1, Post-Gasification (LLL, ERDA) 343

C27 Volatile Organics in Water (-16L) From Dewatering Well #4, Post-Gasification (LLL, ERDA). 344

C28 Volatile Organics in Water (-17L) From Dewatering Well #5, Post-Gasification (LLL, ERDA). 347

C29 Volatile Organics in Water (-18L) From Dewatering Well #4, Post-Gasification (LLL, ERDA). 349

C30 Volatile Organics in Liquid Sample (-19L) From Production Well #1, Post-Gasification (LLL, ERDA) 352

C31 Volatile Organics in Water (-20L) From Production Well #1, Post-Gasification (LLL, ERDA). 353

C32 Volatile Organics in Product Tar (-1L) From In Situ Coal Gasification, Hanna #2, Phase I (LERC, ERDA) 354

C33 Volatile Organics in Ground Water (-2L) From Well #5 Prior to In Situ Coal Gasification (LERC, ERDA). . . . 356

C34 Volatile Organics in Ground Water Sample (-4L) From Well #6 Prior to In Situ Coal Gasification (LERC, ERDA). . . . 357

C35 Volatile Organics in Ground Water (-5L) From Well #5 Prior to In Situ Coal Gasification (LERC, ERDA). 358

TABLES (cont'd)

Number Page

C36 Volatile Organics in Produced Water (-8L) During Well 5-6 *In Situ* Coal Gasification (LERC, ERDA). 360

C37 Volatile Organics in Produced Water (-9L) From Well 5-6 *In Situ* Coal Gasification (LERC, ERDA) 362

C38 Volatile Organics in Product Tar (-10S) From *In Situ* Coal Gasification (LERC, ERDA) 364

C39 Volatile Organics in Product Water #3 (-11L) During Well 5-6 *In Situ* Coal Gasification (LERC). 366

C40 Volatile Organics in Produced Tar (-12T) From Well 5-6 *In Situ* Coal Gasification. 368

C41 Volatile Organics in Produced Water (-13L) From Well 5-6 *In Situ* Coal Gasification (LERC, ERDA) 370

C42 Volatile Organics in Produced Water (-14L) From Well 7-8 *In Situ* Coal Gasification (LERC, ERDA) 373

C43 Volatile Organics in Produced Tar (-15T) From Well 7-8 *In Situ* Coal Gasification (LERC, ERDA) 375

C44 Volatile Organics in Produced Water (-16L) From Well 7-8 *In Situ* Coal Gasification (LERC, ERDA). 379

C45 Volatile Organics in Produced Tar (-17T) From Well 7-8 *In Situ* Coal Gasification (LERC, ERDA) 381

C46 Volatile Organics in Produced Water (-18L) During Well 7-8 *In Situ* Coal Gasification (LERC, ERDA). 385

C47 Volatile Organics in Produced Water (-19L) From Well 7-8 *In Situ* Coal Gasification (LERC, ERDA). 388

C48 Volatile Organics in Ground Water (-20L) From Corehole #3 Post-*In Situ* Coal Gasification (LERC, ERDA) 391

C49 Volatile Organics in Post-Gasification (-21L) from Well #1, Hanna #1 (LERC, ERDA) 393

C50 Volatile Organics in Post-Gasification Water (-221) From Well #8, Hanna 1 (LERC, ERDA) 394

C51 Volatile Organics in Post-Gasification Water (-23L) From Well WQ-1 (LERC, ERDA). 396

C52 Volatile Organics in Post-Gasification Water (-24L) From Well #1, Hanna #2 (LERC, ERDA). 397

TABLES (cont'd)

Number Page

C53 Volatile Organics in Post-Gasification Water (-25L) From Well #4, Hanna II (LERC, ERDA). 400

D1 Semi-Volatile Organics in Liquid Sample From 150 Ton Retort In Situ Oil-Shale Processing (LERC, ERDA) 402

D2 Semi-Volatile Organics in Aqueous Boiler Blow-Down Sample From In Situ Oil-Shale Processing (OCC) 405

D3 Semi-Volatile Organics in Omega-9 Retort Water From In Situ Oil-Shale Processing Prior to Storage at 75°F (LERC, ERDA). 407

D4 Semi-Volatile Organics in Omega-9 Retort Water From In Situ Oil-Shale Processing After Storage at 75°F For 2 Months (LERC, ERDA) 412

D5 Semi-Volatile Organics in Aqueous Condensate (-1L) From Low Btu Gasification of Rosebud Coal (MERC, ERDA) . . . 414

D6 Semi-Volatile Organics in Aqueous Condensate (-2L) From Low Btu Gasification of Rosebud Coal (MERC, ERDA) . . . 416

D7 Semi-Volatile Organics in Tar (-3T) From Knock-Out Chamber During Low Btu Gasification of Rosebud Coal (MERC, ERDA) 418

D8 Semi-Volatile Organics in Aqueous Condensate (-4L) During Low Btu Gasification of Rosebud Coal (MERC, ERDA) . . . 420

D9 Semi-Volatile Organics in Tar (-5T) From Knock-Out Chamber During Low Btu Gasification of Rosebud Coal (MERC, ERDA) 422

D10 Semi-Volatile Organics in Aqueous Condensate (-6L) From Low Btu Gasification of Rosebud Coal (MERC, ERDA) . . . 423

D11 Semi-Volatile Organics in Tar (-7T) From Knock-Out Chamber During Low Btu Gasification of Rosebud Coal (MERC, ERDA) 426

D12 Semi-Volatile Organics in Water (-1L) From Dewatering Well #5 Prior to In Situ Coal Gasificsation (LLL, ERDA). . . 428

D13 Semi-Volatile Organics in Liquid Blend From Dewatering Wells #1 and 6 Prior to In Situ Coal Gasification (LLL, ERDA) 429

TABLES (cont'd)

Number Page

D14 Semi-Volatile Organics in Process Water (-3L) During In Situ Coal Gasification (LLL, ERDA). 430

D15 Semi-Volatile Organics in Process Tar (-4T) From In Situ Coal Gasification (LLL, ERDA). 433

D16 Semi-Volatile Organics in Water (-5L) From Permeation Well #5 (LLL, ERDA). 435

D17 Semi-Volatile Organics in Process Composite (-6L) From In Situ Coal Gasification (LLL, ERDA). 436

D18 Semi-Volatile Organics in Process Composite (-7L) From In Situ Coal Gasification (LLL, ERDA). 440

D19 Semi-Volatile Organics in Water (-8L) From Environmental Monitoring Well #4 During In Situ Coal Gasification (LLL, ERDA). 443

D20 Semi-Volatile Organics in Water (-9L) From Environmental Monitoring Well #5 During In Situ Coal Gasification (LLL, ERDA). 444

D21 Semi-Volatile Organics in Water (-10L) From Dewatering Well #4 (LLL, ERDA). 448

D22 Semi-Volatile Organics in Water (-11L) From Dewatering Well #5 (LLL, ERDA). 450

D23 Semi-Volatile Organics in Water (-12L) From Environmental Monitoring Well #1 After In Situ Coal Gasification (LLL, ERDA). 451

D24 Semi-Volatile Organics in Water (-13L) From Environmental Monitoring Well #4 After In Situ Coal Gasification (LLL, ERDA). 452

D25 Semi-Volatile Organics in Water (-14L) From Environmental Monitoring Well #2 After In Situ Coal Gasification (LLL, ERDA). 453

D26 Semi-Volatile Organics in Liquid (-15T) From Production Well #1 After In Situ Coal Gasification (LLL, ERDA). . 454

D27 Semi-Volatile Organics in Water (-16L) From Dewatering Well #4 After In Situ Coal Gasification (LLL, ERDA). . 455

TABLES (cont'd)

Number Page

D28 Semi-Volatile Organics in Water (-17L) From Dewatering Well #5 After *In Situ* Coal Gasification (LLL, ERDA). . . 456

D29 Semi-Volatile Organics in Water (-18L) From Dewatering Well #4 After *In Situ* Coal Gasification (LLL, ERDA). . . 457

D30 Semi-Volatile Organics in Water (-19L) From Production Well #1 After *In Situ* Coal Gasification (LLL, ERDA). . . 458

D31 Semi-Volatile Organics in Water (-20L) From Production Well #1 After *In Situ* Coal Gasification (LLL, ERDA). . . 459

D32 Semi-Volatile Organics in Tar (-1L) From *In Situ* Coal Gasification During Hanna #2, Phase I (LERC, ERDA) . . . 460

D33 Semi-Volatile Organics in Water (-2L) From Well #5, Hanna #2 (LERC, ERDA). 463

D34 Semi-Volatile Organics in Water (-3L) From Well #6, Hanna #2 (LERC, ERDA) 464

D35 Semi-Volatile Organics in Water (-4L) From Well #6, Hanna #2 (LERC, ERDA) . . . . 46[illegible]

D36 Semi-Volatile Organics in Water (-5L) From Well #5, Hanna #2 (LERC, ERDA) 466

D37 Semi-Volatile Organics in Product Water Sample #1 (-8L) From Well 5-6 *In Situ* Coal Gasification (LERC). 467

D38 Semi-Volatile Organics in Produced Water (-9L) From Well 5-6 *In Situ* Coal Gasification (LERC, ERDA) 468

D39 Semi-Volatile Organics in Tar (-10T) From Well 5-6 *In Situ* Coal Gasification (LERC, ERDA) 469

D40 Semi-Volatile Organics in Produced Water (-11L) From Well 5-6 *In Situ* Coal Gasification (LERC, ERDA) 472

D41 Semi-Volatile Organics in Produced Tar (-12T) From Well 5-6 *In Situ* Coal Gasification (LERC, ERDA) 473

D42 Semi-Volatile Organics in Produced Water (-13L) From Well 5-6 *In Situ* Coal Gasification (LERC, ERDA) 476

D43 Semi-Volatile Organics in Produced Water (-14L) From Well 7-8 *In Situ* Coal Gasification (LERC, ERDA) 477

TABLES (cont'd)

Number Page

D44 Semi-Volatile Organics in Produced Tar (-15T) From Well 7-8 In Situ Coal Gasification (LERC, ERDA) 478

D45 Semi-Volatile Organics in Produced Water (-16L) From Well 7-8 In Situ Coal Gasification (LERC, ERDA). 481

D46 Semi-Volatile Organics in Produced Tar (-17T) From Well 7-8 In Situ Coal Gasification (LERC, ERDA). 483

D47 Semi-Volatile Organics in Produced Water (-18L) From Well 7-8 In Situ Coal Gasification (LERC, ERDA) 486

D48 Semi-Volatile Organics in Produced Water (-19L) From Well 7-8 In Situ Coal Gasification (LERC, ERDA) 487

D49 Semi-Volatile Organics in Water (-20L) From Corehole #3, Post-Gasification (LERC, ERDA). 488

D50 Semi-Volatile Organics in Post-Gasification Water (-21L) From Well #1, Hanna #1 (LERC, ERDA) 492

D51 Semi-Volatile Organics in Post-Gasification Water (-22L) From Well #8, Hanna #1 (LERC, ERDA) 493

D52 Semi-Volatile Organics in Water (-23L) From WQ-1 Post-In Situ Coal Gasification (LERC, ERDA) 494

D53 Semi-Volatile Organics in Post-Gasification Water (-24L) From Well #1, Hanna #2 (LERC, ERDA) 498

D54 Semi-Volatile Organics in Post-Gasification Water (-25L) From Well #4, Hanna #2 (LERC, ERDA) 499

ACKNOWLEDGEMENTS

The valuable assistance of Ms. S. Willis, D. Smith and N. Pardow (RTI) for executing the sample preparation, analysis and data interpretation is gratefully appreciated. Drs. J. T. Bursey, R. A. Jeffcoat, C. M. Sparacino, D. Rosenthal and R. Handy (RTI) provided the expertise for the interpretation of mass spectra and mercury analysis. The helpful suggestions of Dr. M. E. Wall throughout the program are appreciated.

The author wishes also to extend his deep appreciation to Drs. Charles Brandenburg, Bruce King and Dennis Fisher of the Laramie Energy Research Center for valuable discussions and assistance in acquiring the samples from the *in situ* coal gasification process in Hanna, WY. Drs. Richard Poulson and David Farrier of the Laramie Energy Research Center provided samples from the oil-shale processing experiments. A special thanks for their cooperation. The valuable help during the acquisition of samples from *in situ* coal gasification in Gillette, WY by Drs. Douglas Stevens, Jack Campbell and Warren Mead of the Lawrence Livermore Laboratory is gratefully appreciated. Samples provided by the Morgantown Energy Research Center were obtained through the courtesies of C. Shale and A. Moore. I would like to also thank Mr. Terry Thoem of EPA, Region IV, Denver, CO for his assistance and coordination in obtaining a boiler blow-down condensate from the Occidental Oil Company (*in situ* oil-shale processing).

The excellent cooperation by CT&E personnel for providing expedient multi-element analysis throughout the program is appreciated.

The constant encouragement and constructive criticisms of Ms. A. Alford of EPA, Athens, GA are deeply appreciated. All the personnel at EPA who assisted the Project Director by providing information for the state-of-the-art review are acknowledged.

SECTION 1

INTRODUCTION

Our national energy goal is to achieve energy independence for the free world with efficient environmentally safe, clean and acceptable commercialized energy technologies. For the past several years, there has been an increasing concern about the rate of energy consumption within the United States and with the extent to which domestic energy resources can meet these needs. Although estimates vary, it is generally agreed that domestic natural gas supplies and domestic petroleum supplies are sufficient to last for only 15-25 years at the present rates of usage. In contrast, domestic coal reserves are estimated to last for several hundred years and also large resources are available from oil-shale and tar sands. It is evident that the nation's major resource is fossil fuel and that it will be immensely valuable for supplying our nation's energy needs in the future.

It is optimistically anticipated that the production of synthetic fuels will make a significant contribution to energy supplies in the coming years. Recent Energy Research and Development Administration (ERDA) predictions indicate that between 250-500,000 barrels/day of equivalent energy will be produced from coal by 1985. This is equivalent to ~34,000 megawatts of electricity generating capacity.

The Energy Research and Development Administration is charged with the mission for developing the potentially promising coal gasification, liquefaction, oil-shale retorting, etc. systems both within its research centers and national laboratories and in cooperation with industry. One of the large and basic aspects of the assessment of energy conversion is determining what comes out of the process streams in order to identify useful by-products for chemical production so that it can be properly harnessed and to identify toxic or undesirable substances for their control through adequate technological measures.

The expected emphasis on and drive toward national energy self-sufficiency implies a very real possibility for large scale environmental degradation. There is great concern on the one hand that unabated growth in energy production and utilization will cause irreparable harm to the environment and on the otherhand that measures to protect the environment may further exacerbate the current supply problems faced by the energy industry. It is generally recognized that the nation must use coal and oil-shale over the next few decades at a rate of activity which will double or triple our current levels.(1) The research requirements and technology for avoiding serious environmental abuse are vast and range from needed improvements in coal mining and oil-shale processing methods to the problem of disposing of water waste products. Effluents and waste from fuel extraction processing and their use can dangerously affect water quality. This program as well as others, addressed the problem of water contamination from energy-related activities with the major emphasis on the identification of organics and inorganics released to ground water. The data generated from this research program will provide information for future programs about the formation, transportation and degradation mechanisms of chemical elements and organic components of aqueous effluents. Such information developed from this program will provide data to researchers who are concerned with control technology and monitoring techniques in the health and ecological aspects of such energy-related pollution.

Based on the present state of knowledge, one can only make predictions of the probable water pollution problems that will arise in coal and oil-shale conversion processing. The predictions generally could be based upon (a) details of individual conversion processes, including ancillary operations, (b) a knowledge of the organic and inorganic constituents of coal and oil-shale and (c) the geochemistry of the different major coal producing and oil-shale areas of the country.(1) The principal types of minerals in coals are clays, quartz, carbonates and pyrites and sometimes feldspars. Trace and minor elements may be associated with any of these or with the organic matter.(1) The resulting pollution of water may be reflected by the trace and minor elements and organic matter present in the original sample. The state of these elements in the conversion processing will depend upon the nature of the association of each element as well as on its chemical properties.

Oil-shales are widely distributed throughout the United States, but the largest and richest deposit is in the Green River Formation.(2) Thus most efforts to utilize oil-shale have involved material from this formation. The formation covers an area of about 17,000 sq. miles in four principal basins: the Piceance Basin in Colorado, the Unica Basin of Utah and the Washakie and Green River Basins of Wyoming. The Green River formation comprises one of the largest deposits of hydrocarbons in the world and is potentially a source of significant quantities of liquid fuels. Many attempts have been made to mine and retort Green River oil-shale. So far all attempts have been on a pilot plant scale and commercial units are on the drawing board. Five of the more extensive investigations that have been conducted or are being conducted are those by (1) Bureau of Mines, (2) Consolidated group of six oil companies, (3) the Parahoe Development Corporation, (4) Union Oil Company of California and (5) the Colony Development Operation. In addition to the mining and above ground processing, there has been some effort to do in situ retorting.

The three major components of oil-shale production are mining, crushing, and retorting.(1) The facility being planned for the Parachute Creek region by the Colony Development Operation may become a model for oil-shale processing.(1) The Colony Development Operation is a joint venture consisting of four companies, the Oil-Shale Corporation, Shell Oil Company, Ashland Oil Incorporated and Atlantic Richfield Company. Retorting in this development will be accomplished by using the TOSCO II process, a development which began in 1956. In 1965, a 1,000 ton/day semi-works retort was constructed as a full pilot mine on colony property in Middle Park Canyon of Parachute Creek, CO. In the TOSCO II process, crushed raw shale is preheated by dilute phase fluid bed techniques.(1) The production of oil-shale by this retorting process will generate large volumes of waste materials consisting chiefly of spent shale or processed shale. This is a fine black powder-like material in which the dark color is attributed to a small amount of residual carbon which coats the dust particles. The proposed plan will use about 3.3 barrels of water per gallon of major product produced (fuel oil and a special quality liquified petroleum gas).(1) Total water used will be ~175,000 barrels of water per day at a rate of 11 cu ft/sec.

Enviromental effects directly associated with oil-shale processing are expected to result from retort or burnt shale where water has been produced or used in the processors.(1) Retorting oil-shale produces water both from heating the shale and from burning the fuel when the process uses internal combustion. This water will generally be in the range of 3-10 gallons/ton of retorted shale. Because the water has been in contact with the shale oil, it potentially may contain substantial amounts of organic materials. Some studies of this water and suggestions for its treatment have been made.(1,3)

Underground coal gasification (UCG) has been the subject of investigations for more than 100 years.(4) The process has been shown to be technically feasible in several experiments, but previously has been economically unattractive in competition with petroleum resources. The recent development of sources of inexpensive petroleum fuels has resulted in rekindled interest in research on in situ gasification of coals in the United States using modern methods which were not available earlier to other investigators.

Russian activities in underground gasification of coal have been the most sustained.(4) Electricity has been generated from low btu gas in several large scale plants in the Soviet Union from sub-bituminous coals and lignites. Recently, diminished Soviet utilization of UCG for energy production is believed due to the discovery of adequate local petroleum field sources. In England, UCG was studied extensively in field experiments. Production processes that were technically feasible and nearing commercial utilization were abandoned in 1959 because they were not sufficiently economical at that time.(5) Similar investigations were conducted in the United States by the Bureau of Mines from 1946-1959(6-9) and by Gulf Research in 1968.(7) These studies were also discontinued for lack of immediate need and economic factors.

The Bureau of Mines initiated a reassessment of UCG in 1971.(4) This study revealed that a renewed US field effort was appropriate in view of recent advances in drilling technology and instrumentation. A field site near Hanna, WY, was selected and the Hanna 1 experiment was conducted from

March 1973 to March 1974.(12-14) This experiment using the linked vertical well technique demonstrated that western sub-bituminous coals were suited to underground gasification and that the production of 125 btu/cubic foot gas for extended periods of time were possible. The Hanna 1 experiment indicated that in situ instrumentation was necessary to physically and chemically characterize the in situ reaction system and provide sufficient information to allow process control.

A second field experiment, Hanna 2, was thus designed to answer the many questions arising during the Hanna 1 experiment and to include an expanded instrumentation effort. Hanna 2 was conducted in three phases:

Phase I - a preliminary experiment to determine directional in situ permeability to examine the combustion linking of wells, to conduct a limited gasification test and to evaluate instrumentation techniques;

Phase II - a two-well burn to gasify coal between an injection and production well for preparation for the subsequent phase;

and

Phase III - a four-well burn to gasify a square area by adding two injection wells to the pattern prepared by Phase II.

Another UCG program which utilized a unique approach to in situ coal gasification was originated at the Lawrence Livermore Laboratory in 1972.(15-17) This approach used an array of chemical explosives which was detonated to enhance the permeability of a reaction zone within a thick bed of coal. The principal objective was to develop a commercial process for gasifying deep thick western coals to produce pipeline quality gas.

Many of the processes described above which appeared to be promising avenues for the recovery of energy from fossil fuels became incorporated into the current characterization program described in the following sections.

SECTION 2

CONCLUSIONS

A state-of-the-art review was conducted and the information evaluated according to the following criteria: (a) thoroughness of the study, (b) accuracy of sampling techniques used, (c) capability of the instrumental techniques employed; (d) appropiateness of sample purification methods used and (e) completeness of overall quality control measures. Using these criteria, the state-of-the-art review assessment was prepared on organic and elemental components which have been identified in liquid and solid effluents from energy-related processes. The elemental composition samples from these processes was more thoroughly studied by investigators than the organic substances. A paucity of data existed on the organic composition of liquid and solid effluents from oil-shale retorting, in situ oil-shale processing, in situ coal and lignite gasification, coal-fired power plant operation and low btu gasification of coal and lignite. Only meager data were available for the organic composition of liquid and solid wastes from coal processing, oil refinery operation and geothermal activity. Also, very little information was available on the elemental components associated with oil refinery activity. The research conducted to date on the analysis of organics and solid effluents was highly inadequate for the purpose of understanding the efficiency of the energy-related processes and the potential environmental impact. Many of the previous reports conjectured only as to the probable pollutants that would be associated with the energy-related activity. It was concluded that very few significant studies have been conducted on the characterization of the individual organic components in energy-related samples.

The analysis of the energy-related samples for organic components under this program revealed their extreme complexity. The number of components in many of the liquid process samples exceeded 200, which were subsequently identified and quantified utilizing the techniques of inert gas purging and liquid-liquid extraction followed by high resolution glass capillary gas chromatography/mass spectrometry/computer analysis. It was concluded that the analysis of samples from energy-related activities requires very high resolution glass capillary columns, computerized gc/ms/comp and, in addition, the use of ancillary techniques such as gc/ftir/comp to further document and confirm the identity of the organic components in these samples. Sample characterization revealed the presence of many chemical classes including sulfur-containing compounds (thiophenes, mercaptans, sulfides, benzothiazoles, benzothiophenes, etc.), nitrogen-containing compounds (nitriles, pyridines, anilines, quinolines, etc.); oxygen-containing compounds (aldehydes, ketones, acids, phenols, furans, benzofurans, etc.); alkanes, alkenes, aromatics and alkyl aromatics and polynuclear aromatics. The concentrations of the organic constituents in liquid effluents ranged from <1 ppb (~0.01) to several parts-per-thousand in samples taken before and after in situ processes.

The methods employed in this study provided for the analysis of volatile and semi-volatile compounds down to levels of 1 μg/ℓ (1 ppb) and in some cases even lower. Radiolabeled tracer recovery studies indicated quantitative recoveries for volatile compounds with solubilities <2% in water and a boiling point <220°. The procedure was also quantitative for semi-polar compounds with solubilities <10% and boiling points <150°. For highly water soluble compounds (e.g., acetonitrile, formaldehyde, etc.) the purging method was not quantitative. The liquid-liquid extraction and gas chromatographic procedure for semi-volatile compounds gave quantitative recoveries for organic acids, neutral compounds and bases for compounds with boiling points >60° and <270°. Compounds containing zwitterions were not recovered and were not analyzed by these procedures. Compounds with boiling points >275° were not amenable to gas chromatography.

Spark source mass spectrometry and flameless atomic absorption spectrophotometry analysis of liquid influent and effluents from energy-related processes indicated the release of elemental substances with a composition similar to the original fossil fuel matrix.

SECTION 3

RECOMMENDATIONS

Three major phases of research should be expanded and pursued on the characterization of organic and elemental components in effluents from energy-related processes. One major phase should include a continuation of the state-of-the-art summary for the current and past research which has been performed in this area. Specifically, a concerted effort should be devoted to the examination of the open literature for reports on the characterization of organic compounds in energy-related samples. The second major phase should be expanded and intensified studies to characterize the organic content of volatile and semi-volatile compounds in liquid and solid effluents from coal-fired power plants, geothermal processes, lignite gasification processes and oil refineries. It is also recommended that a research program be initiated on the determination of non-volatile organic compounds in liquid and solid effluents as well as the determination of volatile, semi-volatile and non-volatile organic compounds occurring as air emissions.

SECTION 4

PROGRAM OBJECTIVES

The general objectives of this research program were to prepare a state-of-the-art summary of previous research that has addressed the characterization of organic and elemental constituents in effluents from energy-related processes, to select processes needing further study, and to determine the organic and elemental components in effluents from these energy-related processes. The specific aim of the state-of-the-art report was to identify gaps in existing and probable future data on chemical elements and volatile organic compounds in solid waste and aqueous effluents from coal mines, oil refineries, oil-shale processors, coal-fired power plants and coal liquefaction and gasification plants. Based upon this information, the research under this program was to supplement current and completed projects while avoiding duplication of past efforts.

Samples were to be analyzed for elemental components (in duplicate) with a technique capable of detecting and measuring all elements through uranium in the periodic table of elements excepting oxygen, helium, hydrogen, neon, argon, krypton, xenon, radon, nitrogen and carbon. The specific aim was to use a technique that had a minimum detection limit of 2 μg/g for solid waste or 2 μg/ℓ for aqueous effluents and quantitative precision within a factor of 2. The preferred method was spark-source mass spectrometry for all elements except mercury and flameless atomic absorption spectrophotometry for mercury analysis.

Under this program, samples were to be analyzed by gas chromatography in combination with mass spectrometry to identify and measure volatile and semi-volatile organic components present in concentrations of 1 μg/ℓ or greater. One of the major requirements of this project was to use a single analytical protocol to permit comparison among samples and to implement a sound quality control and assurance program.

SECTION 5

STATE-OF-THE-ART REVIEW ON CHARACTERIZATION OF ORGANIC AND ELEMENTAL SUBSTANCES IN ENERGY-RELATED EFFLUENTS

INTRODUCTION

A state-of-the-art summary was prepared to determine which energy-related solid waste and aqueous effluents had been analyzed to identify and quantify specific pollutants and to determine which current contracts and projects would provide further information in this area. The prime objective of this review was to identify gaps in the existing and probable future data on chemical elements and volatile organic compounds in solid waste and aqueous effluents from coal mines, oil refineries, oil-shale processors, coal-fired power plants and coal liquefaction and gasification plants. The information derived from the state-of-the-art review was to serve as a guideline to plan the current program and to supplement current and completed projects occurring in other laboratories.

TECHNICAL APPROACH

Searching and Retrieval Methods

The current literature, contract and technical progress reports were reviewed to obtain and prepare a state-of-the-art summary. The open literature was examined through Chemical Abstracts. Technical reports summarizing the science and technology in this area were obtained by consulting and computer searching of the National Technical Information Service and the Energy Research Information System (Old West Regional Commission and U.S.D.A. Forest Service Surface Environment and Mining, Billings, MN). To obtain information regarding currently funded programs, the Smithsonian Information Exchange was consulted. Other computer retrieval systems such as Medline and Toxline were also used. Finally, personnel were directly contacted at the Environmental Protection Agency, the Energy Research and Development Administration and many non-profit and industrial research organizations.

Evaluation Criteria

The data available in the state-of-the-art review were evaluated according to the following criteria: (a) thoroughness of the study, *i.e.*, the ability to examine and measure the majority, if not all of the components present in waste effluents; (b) sampling techniques; (c) capability of the instrumental techniques employed; (d) sample purification procedures and (e) overall quality control measures.

STATE-OF-THE-ART ASSESSMENT

Appendix A presents abstracts of current projects and reports that were obtained during the information retrieval phase of this program (through December 31, 1976). Tables 1 and 2 summarize the majority of organic and elemental components identified in liquid and solid effluents from energy-related processes. From the number of organic compounds have been identified in oil-shale processing, it was apparent that very little research had been conducted. Two on-going research programs may alleviate this deficiency were those which were under way at the Denver Research Institute in Denver, CO, and a dual venture between Colorado State University and Montana State University. In both programs, the chemical emphasis appears to be on the identification of elemental constituents and polycyclic hydrocarbons in spent shale and aqueous leachates from the above ground retorting operations. A thorough study had not been reported on the composition of product water from *in situ* oil-shale processing.

In contrast, the detection and quantification of elements has been more extensively conducted. An intensive effort to determine elemental components and inorganic compounds in aqueous leachates from spent shale has been conducted. A paucity of information, however, existed on the composition of product water from *in situ* oil-shale gasification.

The identification of organic compounds (Table 1) in tars and chars and in coal preparation, quenching and cooling water in sour aqueous condensates from various coal gasification and liquefaction processes was the most thoroughly examined of the energy-related activities. The gasification liquefaction methods, most studied were the Synthane, Lurgi, K-T, CO_2 acceptor, Hydrane and Solvent Refined Coal (SRC) processes. As indicated by the research reports in Appendix A, extensive research has been conducted on developing and applying analytical techniques for the analysis of organics

Table 1. ORGANIC COMPOUNDS IDENTIFIED IN EFFLUENTS FROM ENERGY-RELATED PROCESSES

	Source of Liquid and Solid Effluents[a]					
Compound of Chemical Class	Oil-Shale Processing	Coal Gasification	Coal Liquefaction	Coal-Fired Power-Plants	Coal Processing	Oil Refineries
Acenaphthalene						L
Acenaphthene		S				L
Acenaphthenols		S				
Acetophenone						L
Acetaldehyde			L		L	
Acetic acid			L			L
Aldehydes						L,S
Alkyl and aromatic hydrocarbons						L,S
Alkyl and aromatic amines					L	
Alkyl and aromatic alcohols						L
Aniline		L,S				
Anthraquinone/Disulfonic acid		L				
Anthracene					S	L
Benzaldehyde		L				
Benzoic acid						L
Benzene		L,S	L		L,S	L
Benzofuranol		L				

(continued)

Table 1 (cont'd)

Compound of Chemical Class	Source of Liquid and Solid Effluents[a] Oil-Shale Processing	Coal Gasification	Coal Liquefaction	Coal-Fired Power-Plants	Coal Processing	Oil Refineries
Benzo(a)anthracene					S	
Benzo(a)anthracene, 7,12-dimethyl	X					
Benzonaphthiothiophenes		S				
Benzonitrile		L				
Benzo(a)pyrene	S				S	
Benzo(e)pyrene					S	
Benzo(g)chrysene					S	
Benzo(g,h,i)perylene	X				S	
Benzo(c)chrysene					S	
Biphenyl					S	
1-Butanol						L
2-Butoxyethanol						L
Carbon disulfide						L
Carbonyl sulfide						L
Carbazoles						L
m-Cresol		L	L		L	L
o-Cresol		L	L		L	L

(continued)

Table 1 (cont'd)

Compound of Chemical Class	Oil-Shale Processing	Coal Gasification	Coal Liquefaction	Coal-Fired Power-Plants	Coal Processing	Oil Refineries
	Source of Liquid and Solid Effluents[a]					
p-Cresol		L	L		L	L
Crysene					S	
Cresylic acid						L
1-Decanol						L
Diacetone alcohol						L
Dibenzofuran		S				L
Dibenzothiophenes		S				
Dibenz(a,h)anthracene					S	
Dibenz(a,j)acridine					S	
Dibenzo(cd, lm)perylene					S	
Dimethyl furan isomer						L
2,6-Dimethylnaphthalene						L
3,3-Diphenylpropanol						L
Dimethylphenol						L
Dodeane						L
Eicosane						L

(continued)

Table 1 (cont'd)

Compound of Chemical Class	Oil-Shale Processing	Coal Gasification	Coal Liquefaction	Coal-Fired Power-Plants	Coal Processing	Oil Refineries
	Source of Liquid and Solid Effluents[a]					
Ethylene glycol		L				
Ethyl naphthalene						L
o-Ethyltoluene						L
Fluorene		S			S	
Formaldehyde			L		L	
Fluoranthrene	X				S	
Furans					L	
Formic acid						L
Heneicosane						L
Heptadecane						L
Hexadecane						L
1-Hexanol						L
Indane		S				L
Indanols		S				
4-Indanol		S				
Indene		S				L

(continued)

Table 1 (cont'd)

Compound of Chemical Class	Source of Liquid and Solid Effluents[a]					
	Oil-Shale Processing	Coal Gasification	Coal Liquefaction	Coal-Fired Power-Plants	Coal Processing	Oil Refineries
Indole		S				
Maleic anhydride						L
Maleic acid						L
m-Methoxyindole		S				
α-Methylbenzyl alcohol						L
Methyl biphenyl isomer						L
Methyl ethyl naphthalene isomer						L
1-Methyl indene						L
3-Methyl indene						L
1-Methylnaphthalene						L
2-Methylnaphthalene						L
Methyl indole		L				
Methyl mercaptan		L,S				L,S
Methyl anilines					L	
o-Methylstyrene						L
β-Methylstyrene						L

(continued)

Table 1 (cont'd)

Compound of Chemical Class	Source of Liquid and Solid Effluents[a]					
	Oil-Shale Processing	Coal Gasification	Coal Liquefaction	Coal-Fired Power-Plants	Coal Processing	Oil Refineries
Naphthalene		L,S	L			L
Naphthols		S				
1-Naphthol		L				
2-Naphthol		S				
Naphthol, methyl		L				
Nonadecane						L
1-Octanol						L
Octadecane						L
Oleic acid						L
Phenanthrene		L				
Phenanthrols		S				
Phenol		L,S	L		L,S	L
o-Ethylphenol		L				
p-Ethylphenol		L				
o-Isopropylphenol		L				
2-Methyl-4-ethylphenol		L				

(continued)

Table 1 (cont'd)

Compound of Chemical Class	Source of Liquid and Solid Effluents[a] Oil-Shale Processing	Coal Gasification	Coal Liquefaction	Coal-Fired Power-Plants	Coal Processing	Oil Refineries
3-Methyl-6-ethylphenol		L				
4-Methyl-2-ethylphenol		L				
2,3,5-Trimethylphenol		L				
1-Phenylnaphthalene		S				
Pyridine		L,S			L	L
Pyridine, ethyl		L				
Pyridine, methyl		L				
Pyrroles						L
Pyrene	X				S	
Pyrocatechol		L,S				
Pyrocatechol, methyl		L				
Palmitic acid						L
Pentadecane						L
Quinolines						L
Styrene						L
Thiophene		L,S	L		L	L

(continued)

Table 1 (cont'd)

Compound of Chemical Class	Source of Liquid and Solid Effluents[a] Oil-Shale Processing	Coal Gasification	Coal Liquefaction	Coal-Fired Power-Plants	Coal Processing	Oil Refineries
Thiophene, dimethyl		L,S				
Thiophene, methyl		L,S	L			
Toluene		L,S	L		L	L
Thiosulfide						L
α-Terpineol						L
Tetradecane						L
n-Tridecane						L
Undecane						L
Xylene (o,m,p)			L		L	L
2,3-Xylenol		L				
2,4-Xylenol		L				
2,5-Xylenol		L				
2,6-Xylenol		L				
3,4-Xylenol		L				
3,5-Xylenol		L				
γ-valerolactones	L					

(continued)

Table 1 (cont'd)

Compound of Chemical Class	Source of Liquid and Solid Effluents[a]					
	Oil-Shale Processing	Coal Gasification	Coal Liquefaction	Coal-Fired Power-Plants	Coal Processing	Oil Refineries
Sulfides						L,S
Sulfites						L,S
Sulfonates						L,S
Sulfones						L,S

[a] L = liquid, S = solid effluents

Table 2. ELEMENTAL COMPOUNDS IDENTIFIED IN EFFLUENTS FROM ENERGY-RELATED PROCESSES

	Source of Liquid and Solid Effluents[a]					
Elemental or Inorganics	Oil-Shale Processing	Coal Gasification	Coal Liquefaction	Coal-Fired Power-Plants	Coal Processing	Oil Refineries
Au				L,S	S	
Ag				L,S	S	
Al	L,S	L		L,S	S	
Al_2O_3	X	S		L,S	S	
Ammonia		L	L			
Ammonium cyanate			L			
As	S	L,S		L,S	L,S	
Arsenic acid, Na salt		L	L			
Ar_2O_2		L	L			
Arsine		L				
Ba	L,S	L	L	L,S	L,S	L
$BaCl_2$			L			
Be	S	L,S		L,S	S	
Bi				L,S	S	
B		L,S		L,S	S	

(continued)

Table 2 (cont'd)

	Source of Liquid and Solid Effluents[a]					
Elemental or Inorganics	Oil-Shale Processing	Coal Gasification	Coal Liquefaction	Coal-Fired Power-Plants	Coal Processing	Oil Refineries
BO		S				
Br_2		L			S	
Ca	S	L	S	L,S		
$CaCl_2$			L,S			
CaO		L			S	
$CaSO_4$			L,S			
CaS		S				
Cd	L,S	L,S	L	L,S	L,S	
$CdCl_2$			L			
$CdNO_3$			L			
Ce	S			L,S	S	
Cs				L,S	S	
CS_2		L,S				
COS		L	L			
Cl_2		L		L,S	S	

(continued)

Table 2 (cont'd)

Elemental or Inorganics	Source of Liquid and Solid Effluents[a]					
	Oil-Shale Processing	Coal Gasification	Coal Liquefaction	Coal-Fired Power-Plants	Coal Processing	Oil Refineries
Cr	L,S	L,S	S	L,S	S	
Co	S	L		L,S	S	S
Cobalt Molybdate			S			
Cu	L,S	L		L,S	S	L,S
Cyanides		L	L			
Dysorium	S			L,S	S	
Erbuim				L,S	S	
Europuin	S			L,S	S	
Fe	L,S	L		L,S		
FeCl$_3$	L	S				
F		L	L	L,S	S	
Ge		L		L,S	S	
Gadolinium				L,S	S	
Ga	S			L,S	S	
Hafnium	S			L,S	S	
Holmiun				L,S		

(continued)

Table 2 (cont'd)

Elemental or Inorganics	Oil-Shale Processing	Coal Gasification	Coal Liquefaction	Coal-Fired Power-Plants	Coal Processing	Oil Refineries
	Source of Liquid and Solid Effluents[a]					
HCl		L				
HCN		L,S	L			
HF		L				
H_2S		L	L			
Hg	S	L,S	L	L,S	L,S	
K	L,S	L			S	
La	S				S	
Li	S				S	
Mg	S	L			S	
$MgCl_2$			L,S	L,S		
MgO	X	L				
Mn	L,S	L		L,S	S	
Mo				L,S	S	S
Na	S	L,S	L,S	L,S	S	S
Nb					S	
Ni	L	S		L,S	S	L,S

(continued)

Table 2 (cont'd)

	Source of Liquid and Solid Effluents[a]					
Elemental or Inorganics	Oil-Shale Processing	Coal Gasification	Coal Liquefaction	Coal-Fired Power-Plants	Coal Processing	Oil Refineries
NiCO		L			L	
P	S	L			L,S	
Pb	L,S	L,S	L	L,S	S	
Rb	S					
Sa	S					
Sb	S	L,S	L	L,S	S	
Sc	S				S	
Se		L,S	L	L,S	L,S	
Sn		L			S	
Sr	S	L			S	L
Te		L			S	
Th	S					
Ti	S			L,S	S	
Tl	S					
U	S				S	
V	S	L,S	L	L,S	S	L,S

(continued)

Table 2 (cont'd)

	Source of Liquid and Solid Effluents[a]					
Elemental or Inorganics	Oil-Shale Processing	Coal Gasification	Coal Liquefaction	Coal-Fired Power-Plants	Coal Processing	Oil Refineries
V_2O_5		L	L,S			
Y					S	
Zn	L,S	L,S	L	L,S	S	L,S
ZnO		S			S	
Zr					S	

[a] L = liquid, S = solid effluents

(principally gas chromatography/mass spectrometry) in liquid and solid materials from these processes.

Likewise, a major effort had been devoted to the detection and measurement of elemental components in liquids and solids from coal gasification and liquefaction. The predominant characterization effort had addressed the Synthane and high-btu methods. Less information was available from the low btu coal and lignite gasification techniques. In contrast, the characterization and quantification of organic and elemental constituents in the product water from in situ coal gasification had not been conducted.

Thorough analysis for organic compounds in fly ash, bottom ash and quenching and cooling water from coal-fired power plants had not been conducted (Table 1). However, work had been performed on elemental components in liquids and solids (Table 2). The Radian Corporation had executed a material balance study for three coal-fired power plants. This study appears to be one of the best efforts on elemental analysis utilizing modern analytical techniques.

Waste materials associated with coal processing, e.g., mine dust, coal leachates or mine spoilage from natural water runoff has also been examined. Reports on qualitative analysis of organic constituents by gas chromatography/mass spectrometry and elemental components by spark source mass spectrometry are included in Appendix A.

Cooling water, quench water, sour aqueous discharge spent acid sludge and spent catalyst from oil refinery processes have been studied and many organics (Table 1) have been reported. Additional research appears to be necessary, however, for those processes utilizing high sulfur content oils and coals, particularly with respect to elemental analysis.

In summary, a paucity of data existed on the organic composition of liquid and solid effluents from oil-shale retorting, in situ oil-shale processing in situ coal and lignite gasification, coal-fired power plants, and low btu gasification of coal and lignite. Meager data were available for the organic composition of liquids and solids from coal processing, oil refinery operation and geothermal activity. Also, very little information was available on elemental components associated with oil refinery activity. In general it was concluded that the research conducted to date on the analysis for organics in liquid and solid effluents was highly inadequate for the purpose of understanding the efficiency of the energy-related processes and the potential environmental impact. Much of the data were based on "paper" studies that merely conjectured as to the probable pollutants that would be associated with the energy-related activity. When evaluating the available data on the elemental and organic composition of effluents from energy-related processes according to the criteria previously described--particularly the thoroughness of the study and its ability to provide specific individual chemical information for all the species present in the effluents--we found few significant energy-related studies.

Appendix A, Section I contains abstracts of technical reports and current projects on oil-shale processing, Section II-coal gasification and liquefaction, Section III-coal-fired power plants, Section IV-coal related pollution, Section V-oil refineries and Section VI-tar sands.

SECTION 6

SAMPLES AND SAMPLING PROCEDURE

INTRODUCTION

In view of the paucity of data on the individual species of organic and elemental constituents in liquid and solid effluents from in situ coal gasification and oil-shale retorting uncovered during the state-of-the-art summary, these energy-related areas were selected for study. In conjunction with the EPA Project Officer, RTI contacted personnel at two Energy Research and Development Administration research centers (Laramie Energy Research Center, LERC, and Lawrence Livermore Laboratory, LLL) to establish cooperative agreements for collecting and analyzing samples from in situ coal gasification processes occurring in Hanna and Gillette, WY, respectively. Liquid and solid samples from an oil-shale retorting process in Debeque, CO, were also obtained. Samples from oil-shale retorting systems were also obtained from LERC.

A cooperative study was also established with the Morgantown Energy Research Center (MERC) for the purpose of examining liquid and tar effluents from a low btu coal gasification system.

The oil-shale and coal gasification experiments conducted under the auspices of ERDA have been previously described.(15-18)

SAMPLING TECHNIQUES

Preparation of Sampling Containers

Glass sampling containers were cleaned with dilute mineral acid (HCl), rinsed with deionized-distilled water and then placed in an oven at 450°C for 2 hr to remove any organic material. Teflon-lined, septum-type caps without adhesives were utilized in order to minimize the inherent problem of contamination.

Sample Containers, Shipment and Storage

Samples designated for spark-source mass spectrometry were placed in plastic bottles provided by Commercial Testing & Engineering Co. (CT&E, Golden, CO): these containers were specially cleaned prior to receiving samples by CT&E.

One-liter glass amber bottles (narrow mouth) were used for the collection, transportation and storage of liquid samples designated for analysis of organic compounds; a 32-oz (wide-mouth) glass amber bottle was used for the collection of tar and solid waste materials.

From the standpoint of time of transit, the preferred means of shipment was Federal Express. This carrier was used for shipment of containers from the laboratory to the field sites and for return of the samples; delivery of materials was completed within a 24 hr period. The glass amber bottles were placed in custom-made styrofoam lined shipping containers (Hibco Plastics Co., Yadkinville, NC).

For quality control purposes personnel from RTI were present at the field sites to instruct ERDA personnel on the collection of samples at the beginning of each of the experiments. Well water samples obtained from the Hanna *in situ* coal gasification site were retrieved using a brass bailer. Samples designated for elemental analysis were obtained using a lucite bailer. Product water and tar from the *in situ* coal gasification (Hanna) was obtained from the product stream using a heat-exchange method. The method used for sampling the high temperature stream utilized an ethylene-glycol-cooled condenser system. The condensate from the stream was collected directly in a sump where the product tar and water separated and then placed in the glass amber bottles for later analysis. The entire heat exchange sampling system was constructed of stainless steel material.

Samples from the low btu coal gasification process were taken directly from the knock-out chamber.

Quality Control

Prior to shipment to the field site, sampling containers were checked for potential contamination. Generally one or two containers were filled with deionized distilled water, transported to the field and returned and analyzed to determine the potential contamination from the shipping, storage and sample preparation methods.

During sample collection, a sample data sheet was attached to each container prior to shipment to the RTI laboratory. The coded form (in duplicate) contained information such as date and time of sampling, origin of effluent waste relative to the energy-related process (e.g., product water or tar, in situ coal gasification, etc.), method of sample acquisition (from sump, knock-out chamber, etc.) and whether the sample represented composite or accumulated material. Upon arrival at the RTI laboratory, the samples were logged in by date received and separated according to energy process type. A separate log book was maintained containing information as a running account of sample preparation, analysis and data interpretation.

Samples (in duplicate) designated for multi-element analysis were coded in alphabetic/numeric form and submitted on a blind basis to CT&E for analysis.

Samples Received

Table 3 presents a description of the energy-related liquid and solid effluents received and characterized for elemental and organic substances. These samples were submitted to the analysis procedures described in Section 7.

Table 3. DESCRIPTION OF ENERGY-RELATED LIQUID AND SOLID EFFLUENTS RECEIVED AND CHARACTERIZED FOR ELEMENTAL AND ORGANIC SUBSTANCES

Energy-related Activity	Organization	Processing Site	Sample Type	Sampling Date	Sample Code
In-situ Oil-Shale Processing	Occidental Oil Shale, Inc.	DeBeque, CO	Boiler blown-down water	3/17/76	
In-situ Oil-Shale Processing	Occidental Oil Shale, Inc.	DeBeque, CO	Discarded cavern oil-shale	3/17/76	
In-situ Oil-Shale Processing	LERC (ERDA)		Oil-shale formation water		
In-situ Oil-Shale Processing	LERC (ERDA)	Rock Springs, WY	OMEGA-9 retort water	Sept.-Oct., 1976	
In-situ Coal Gasification	LERC (ERDA)	Hanna, WY	Product water sample from Hanna II, Phase I experiment		100ICG-1L
In-situ Coal Gasification	LERC (ERDA)	Hanna, WY	Ground water sample, well #5, Hanna II, prior to gasification water level was 256 ft.	3/18/76	200ICG-2L
In-situ Coal Gasification	LERC (ERDA)	Hanna, WY	Ground water sample, well #6, Hanna II, prior to gasification water level was 180 ft.	3/18/76	200ICG-3L
In-situ Coal Gasification	LERC (ERDA)	Hanna, WY	Ground water sample, well #6, Hanna II, prior to gasification water level was 201 ft.	3/25/76	300ICG-4L
In-situ Coal Gasification	LERC (ERDA)	Hanna, WY	Ground water sample, well #5, Hanna II, prior to gasification water level was 302 ft.	3/25/76	300ICG-5L
In-situ Coal Gasification	LERC (ERDA)	Hanna, WY	Deionized/distilled water in bailer for 10 min., used as reference.	3/25/76	300ICG-6L
In-situ Coal Gasification	LERC (ERDA)	Hanna, WY	Deionized/distilled water blank for bailer.	3/25/76	300ICG-7L
In-situ Coal Gasification	LERC (ERDA)	Hanna, WY	Product water sample from Hanna II, well 5-6 gasification.	4/26/76 (1400 hr)- 4/27/76 (2200 hr)	400ICG-8L
In-situ Coal Gasification	LERC (ERDA)	Hanna, WY	Product water sample from Hanna II, well 5-6 gasification.	5/5/76 (1000 hr)- 5/7/76 (0900 hr)	500ICG-9L
In-situ Coal Gasification	LERC (ERDA)	Hanna, WY	Product tar sample from Hanna II, well 5-6 gasification.	5/5/76 (1000 hr)- 5/7/76 (0900 hr)	500ICG-10S
In-situ Coal Gasification	LERC (ERDA)	Hanna, WY	Product water sample from Hanna II, well 5-6 gasification.	5/18/76 (0900 hr)- 5/19/76 (0700 hr)	600ICG-11L
In-situ Coal Gasification	LERC (ERDA)	Hanna, WY	Product tar sample from Hanna II, well 5-6 gasification.	5/18/76 (0900 hr)- 5/19/76 (0700 hr)	600ICG-12S
In-situ Coal Gasification	LERC (ERDA)	Hanna, WY	Product water sample from Hanna II, well 5-6 gasification.	5/21/76 (0900 hr)- 5/21/76 (1900 hr)	600ICG-13L
In-situ Coal Gasification	LERC (ERDA)	Hanna, WY	Product water sample from Hanna II, well 7-8 gasification.	7/6/76 (0130 hr)- 7/7/76 (0900 hr)	700ICG-14L
In-situ Coal Gasification	LERC (ERDA)	Hanna, WY	Product tar sample from Hanna II, well 7-8 gasification.	7/6/76 (0130 hr)- 7/7/76 (0900 hr)	700ICG-15S

(continued)

Table 3 (cont'd)

Energy-related Activity	Organization	Processing Site	Sample Type	Sampling Date	Sample Code
In-situ Coal Gasification	LERC (ERDA)	Hanna, WY	Product water sample from Hanna II, well 7-8 gasification.	7/8/76 (0700 hr)- 7/9/76 (0800 hr)	700ICG-16L
In-situ Coal Gasification	LERC (ERDA)	Hanna, WY	Product tar sample from Hanna II, well 7-8 gasification.	7/8/76 (0700 hr)- 7/9/76 (0800 hr)	700ICG-17S
In-situ Coal Gasification	LERC (ERDA)	Hanna, WY	Product water sample from Hanna II, well 7-8 gasification.	7/14/76 (2200 hr)- 7/15/76 (2300 hr)	800ICG-18L
In-situ Coal Gasification	LERC (ERDA)	Hanna, WY	Product water sample from Hanna II, well 7-8 gasification.	7/16/76 (2100 hr)- 7/17/76 (2100 hr)	800ICG-19L
In-situ Coal Gasification	LERC (ERDA)	Hanna, WY	Ground water from corehole #3, water level 116 ft.	11/8/76	900ICG-20L
In-situ Coal Gasification	LERC (ERDA)	Hanna, WY	Post-gasification water sample from well #1, Hanna I water level was 117 ft.	11/8/76	900ICG-21L
In-situ Coal Gasification	LERC (ERDA)	Hanna, WY	Post-gasification water sample from well #8, Hanna I water level was 107 ft.	11/8/76	900ICG-22L
In-situ Coal Gasification	LERC (ERDA)	Hanna, WY	Post-gasification water sample from WQ-1 water level was 239 ft.	11/8/76	900ICG-23L
In-situ Coal Gasification	LERC (ERDA)	Hanna, WY	Post-gasification water sample from well #1, Hanna II water level was 184 ft.	11/8/76	900ICG-24L
In-situ Coal Gasification	LERC (ERDA)	Hanna, WY	Post-gasification water sample from well #4, Hanna II water level was 165 ft.	11/8/76	900ICG-25L
Low-btu Coal Gasification	MERC (ERDA)	Morgantown, WV	Aqueous condensate from gasification of Rosebud coal.	7/22/76	103CGC-1L
Low-btu Coal Gasification	MERC (ERDA)	Morgantown, WV	Aqueous condensate from gasification of Rosebud coal.	7/23/76	103CGC-2L
Low-btu Coal Gasification	MERC (ERDA)	Morgantown, WV	Aqueous condensate from gasification of Rosebud coal.	7/23-24/76	103CGC-3L
Low-btu Coal Gasification	MERC (ERDA)	Morgantown, WV	Aqueous condensate from gasification of Rosebud coal.	7/28/76	103CGC-4L
Low-btu Coal Gasification	MERC (ERDA)	Morgantown, WV	Tar condensate from knock-out chamber from gasification of Rosebud coal.	7/23/76	103CGC-5T
Low-btu Coal Gasification	MERC (ERDA)	Morgantown, WV	Tar condensate from knock-out chamber from gasification of Rosebud coal.	7/27/76	103CGC-6T
Low-btu Coal Gasification	MERC (ERDA)	Morgantown, WV	Tar condensate from knock-out chamber from gasification of Rosebud coal.	7/28/76	103CGC-7T

(continued)

Table 3 (cont'd)

Energy-related Activity	Organization	Processing Site	Sample Type	Sampling Date	Sample Code
In-situ Coal Gasification	LLL (ERDA)	Gillette, WY	Aqueous sample from dewatering well #5	10/25/76	104ICG-1L
In-situ Coal Gasification	LLL (ERDA)	Gillette, WY	Blend of liquids from dewatering well #1 and 6	10/25/76	104ICG-2L
In-situ Coal Gasification	LLL (ERDA)	Gillette, WY	Process water from *in-situ* coal gasification	10/25/76	104ICG-3L
In-situ Coal Gasification	LLL (ERDA)	Gillette, WY	Process tar from *in-situ* coal gasification	10/25/76	104ICG-4L
In-situ Coal Gasification	LLL (ERDA)	Gillette, WY	Well water sample from perm #5	10/25/76	104ICG-5L
In-situ Coal Gasification	LLL (ERDA)	Gillette, WY	Liquid process composite	10/25-26/76	204ICG-6L
In-situ Coal Gasification	LLL (ERDA)	Gillette, WY	Liquid process composite	10/25-26/76	204ICG-7L
In-situ Coal Gasification	LLL (ERDA)	Gillette, WY	Water sample from environmental well #4	11/1/76	204ICG-8L
In-situ Coal Gasification	LLL (ERDA)	Gillette, WY	Water sample from environmental well #5	11/1/76	204ICG-9L
In-situ Coal Gasification	LLL (ERDA)	Gillette, WY	Water sample from dewatering well #4	11/1/76	204ICG-10L
In-situ Coal Gasification	LLL (ERDA)	Gillette, WY	Water sample from dewatering well #5	11/1/76	204ICG-11L
In-situ Coal Gasification	LLL (ERDA)	Gillette, WY	Water sample from environmental monitoring well #1 (30.5 m from burn zone) prior to taking sample, well was pumped for 1 hr. @ 28-56 l/min.	1/18/77	304ICG-12L
In-situ Coal Gasification	LLL (ERDA)	Gillette, WY	Water sample from environmental monitoring well #4 (15 m from burn zone) prior to taking sample, well was pumped for 1 hr. @ 28-56 l/min.	1/18/77	304ICG-13L
In-situ Coal Gasification	LLL (ERDA)	Gillette, WY	Water sample from environmental monitoring well #2 (30.5 m from burn zone) prior to taking sample, well was pumped for 1 hr. @ 28-56 l/min.	1/18/77	304ICG-14L
In-situ Coal Gasification	LLL (ERDA)	Gillette, WY	Tar sample from "Production Well #1", tar was was floating on standing water.	1/19/77	304ICG-15L
In-situ Coal Gasification	LLL (ERDA)	Gillette, WY	Water sample from dewatering well #4, 1 hr. after pumping @ 28-56 l/min.	1/19/77	304ICG-16L
In-situ Coal Gasification	LLL (ERDA)	Gillette, WY	Water sample from dewatering well #5, 1 hr. after pumping @ 84 l/min	1/20/77	304ICG-17L
In-situ Coal Gasification	LLL (ERDA)	Gillette, WY	Initial liquid sample from dewatering well #4, prior to any pumping.	1/19/77	304ICG-18L
In-situ Coal Gasification	LLL (ERDA)	Gillette, WY	Liquid sample from production well #1, 70 min. after pumping @ 84 l/min.	1/20/77	304ICG-19L
In-situ Coal Gasification	LLL (ERDA)	Gillette, WY	Liquid sample from production well #1, after over 1 hr. of pumping.	1/20/77	304ICG-20L

SECTION 7
PHYSICAL METHODS OF ANALYSIS

ELEMENTAL CONSTITUENTS

Mercury Determination by Flameless Atomic Absorption

The total mercury content in samples of process water, tar, oil etc. was determined by flameless atomic absorption spectrophotometry. The analytical protocol was based upon the method described by Kubasik.(19)

SAMPLE PREPARATION

Solid Material

All solid waste samples were submitted to a preliminary treatment to yield powders with a mesh size of 200-325. When required, collected materials were crushed and finely ground to 200-325 mesh using a micromill.(20) Solid samples were air-dried and treated similarly.

Solid samples were digested in a Teflon-lined Parr Model 4745 acid digestion bulb.(21,22) This technique prevented the loss of volatile mercury compounds. Organic compounds were digested by treating with fuming nitric acid and the silaceous material dissolved with hydrofluoric acid. A 50-100 mg sample was typically treated with 2-5 ml of fuming nitric acid in a closed bomb at 150°C for 2.5 hr. After cooling the bomb, 2-5 ml of hydrofluoric acid was added. Additional heating of the powder bomb at 150°C for 15 min was applied, then the powder bomb was cooled to ambient temperatures and the contents transferred to a 50-ml pyrex volumetric flask containing dilute boric acid solution. The final mixture was diluted to a known volume and stored in polyethylene bottles until ready for analysis.

Aqueous Samples

No digestion of sample was required; however, to prevent the adsorption of mercury to container walls, 50 µℓ of a solution containing 5 ml of concentrated nitric and 500 mg of potassium dichromate was added to a 10-ml sample. This quantity was sufficient to decompose the organic materials.

The final mixtures were diluted to a known volume and stored in polyethylene bottles until they were ready for analysis.

Tar/Oil Samples

A wet oxidation decomposition procedure was used for the analysis of mercury in tar/oil samples. The digestion apparatus consisted of a 500 ml two-neck flask; a 75 ml distillation receiver equipped with a 2.5 mm o.d. medium wall side-arm and a two-way teflon stopcock; a 60-ml addition funnel and a 300 ml Friedrichs condenser. All ground glass joints were lubricated with concentrated sulfuric acid. Twenty-five milliliters of concentrated sulfuric acid was added to 5 g of the sample in the digestion apparatus. The solution was stirred and 50-ml of concentrated nitric acid was added dropwise through the addition funnel. After the addition of nitric acid was complete, the temperature was gradually raised and the solution was refluxed for 1 hr until fumes of nitrogen oxide ceased to evolve. The mixture was evaporated down to the fumes of sulfuric acid and then the volatile components were collected in the distillation receiver. The residue was fumed for 5 min and then 25 ml of concentrated nitric acid was added dropwise. The distillate was collected until all the nitric acid had been added and fumes of sulfuric acid were generated in the flask. The solution was allowed to fume for 5 min. The distillate was returned dropwise to the flask and after all the distillate had been returned, it was refluxed for 15 min. The distillation procedure was repeated once more and the solution was then allowed to cool. The interior of the condenser and the distillation receiver was washed with ~100 ml of water. The washings were collected in the flask. The solution was then extracted with three 100-ml portions of n-hexane to remove water insoluble undigested organic matter. Nitrogen was bubbled through the extracted solution until no bubbles of n-hexane were visually observed. A prolonged sweeping of the mixture with nitrogen was avoided to minimize mercury loss. Twenty milliliters of solution containing 12 g of NaCl and 12 g of hydroxylamine sulfate in 100 ml of water was added dropwise with stirring. Stirring was continued until the evolution of gas ceased and then the air space was swept with nitrogen. The sample was then ready for analysis.

SAMPLE ANALYSIS

Solid waste, aqueous and tar/oil samples that were prepared by the above procedures were analyzed with a Perkin-Elmer Model 403 atomic absorption spectrometer equipped with a mercury hollow cathode lamp and a Perkin-Elmer Model 56 recorder as the measuring device. The atomic absorption spectrometer was equipped with a deuterium arc background corrector. A mercury sampling system similar to that described by Kubasik, et al.(19) was used without the magnesium perchlorate drying tube.

The instrumental parameters in Table 4 were used.

Table 4. INSTRUMENTAL OPERATING PARAMETERS FOR FLAMELESS ATOMIC ABSORPTION SPECTROPHOTOMETER

Parameter	Setting
Spectrophotometer/Recorder	
Slit	x 2
Recorder full scale	1A
Recorder response	x 2
Wavelength	253.7 nm
Lamp Current	10 mA
Absorption cell	153 mm long
Chart speed	10 mm/sec
Scale setting	1 mV
Purge gas (N_2)	
Cylinder pressure	50 psi
Flow rate	1 ℓ/min

To a 16 x 100 ml vacutainer tube (No. L3200-4807 Becton-Dickinson & Co., Rutherford, NJ) was added 1 ml of sample and 0.5 ml of concentrated H_2SO_4. The contents were cooled in ice and to them was added 3.5 ml of a 6% potassium permanganate solution. The tubes were covered with parafilm and held at ice temperatures overnight.

The tube was centrifuged and a 1-ml aliquot of the supernatant was transferred to another vacutainer. The tube was connected to the mercury analysis system and 1.0 ml of a stannous chloride solution (200 g/ℓ in 6M

HCl) was introduced through the vacutainer stopper in a 1-ml detachable syringe. The solution was immediately vortexed on a Vortex genie for 15 sec. With a purge gas in a by-pass position, the stopcock controlling the direction of the nitrogen flow was rotated to 180°, flushing the mercury vapor space through the absorption cell. The absorbance was recorded and the system readied for another sample.

Each sample was digested in duplicate and at least 1 ml aliquots were analyzed from each digest. The blank and all standards were analyzed in the same manner.

Standard solutions were made up in the following manner:

(1) 1 ml of a 1,000 ppm mercury standard solution (Fisher Scientific Co.) was diluted in a volumetric flask with deionized water. Final concentration was 10 µg/ml;

(2) 1 ml of the above solution was diluted to 100 ml in a volumetric flask with deionized water, final concentration 100 ng/ml;

(3) to each of six vacutainers were added 1 ml of deionized water and 0.5 ml of concentrated H_2SO_4 with ice cooling. Increasing amounts of mercury solution was added to the tubes. Each standard solution was made up in duplicate;

(4) to each tube was added 3.5 ml of 6% potassium permanganate solution, the top covered with parafilm and held at ice bath temperatures overnight;

(5) two 1 ml aliquots of these solutions were analyzed as described above;

(6) an average peak height was determined for each mercury concentration and after correcting for the blank volume plotted on linear graph paper against mercury concentration. A typical calibration curve is shown in Fig. 1. Mercury concentrations in samples were interpreted directly from this plot.

DETECTION LIMITS

The analytical protocol was capable of analyzing mercury with detection limits of 0.4 ng/ml. For solids, a detection limit of 2 µg/g was typical. A 100-mg sample with this concentration corresponded to a digested solution of 0.2 µg/50 ml (4 ng/ml). The detection limits for tar samples were somewhat higher and were highly dependent upon the background contribution from the sample from other constituents present.

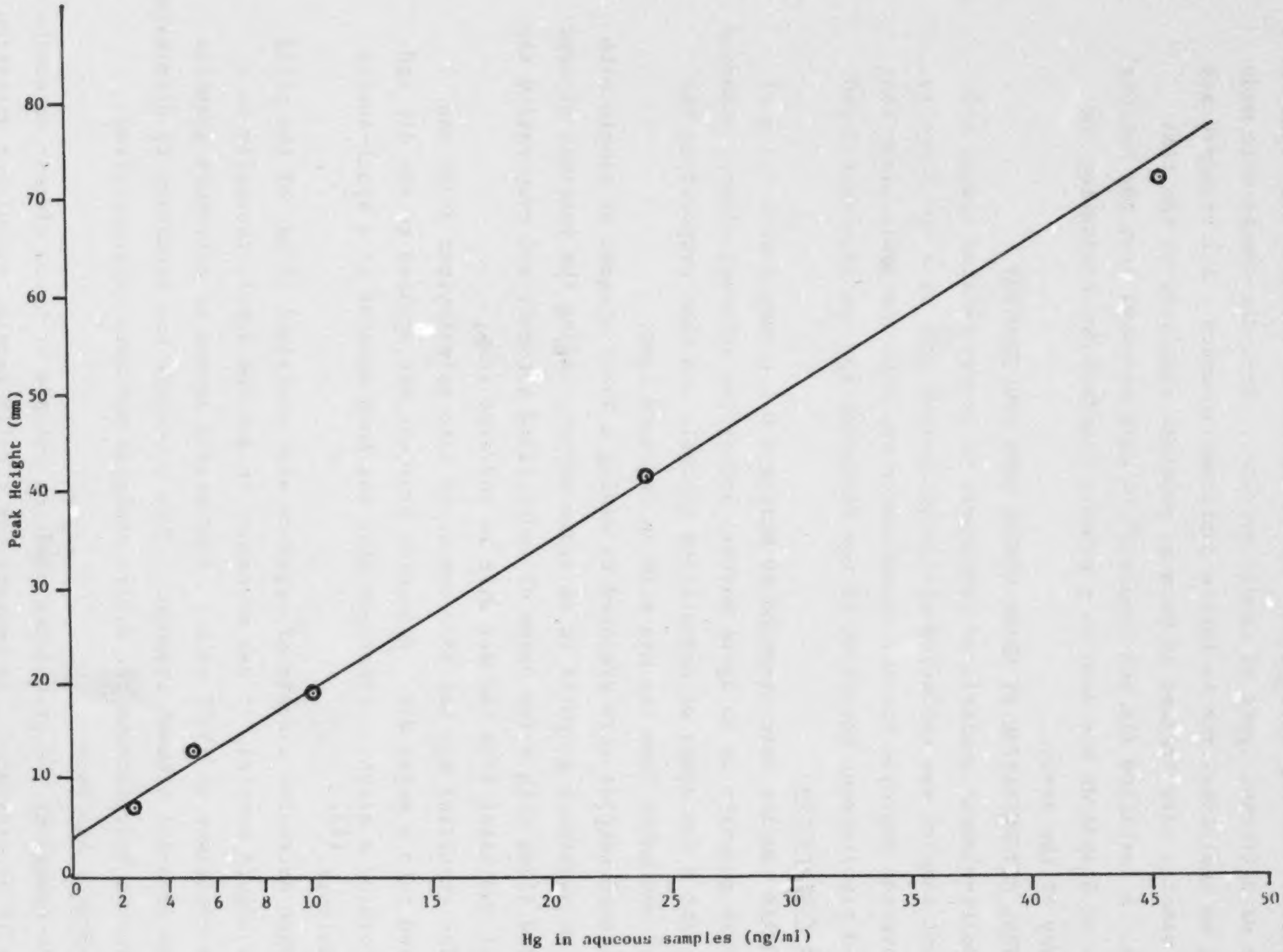


Figure 1. Calibration curve for total mercury analysis in aqueous samples.

INSTRUMENT CALIBRATION (QUALITY CONTROL)

Calibration was accomplished by the method of standard additions for a number of different types of sample matrices. Periodic checks were made during an analytical run to insure continued accuracy. All standard and blank samples were treated as much as possible similarly to the test sample. A certified fly ash sample (0.14 μg/g mercury) from the National Bureau of Standards was used as a primary standard for evaluating the accuracy of the assay.

ELEMENTAL DETERMINATION BY SPARK-SOURCE MASS SPECTROMETRY

Multi-element analysis of components of energy-related wastes and effluent samples was conducted utilizing spark-source mass spectrometry. The detector employed for the spark-source was a photographic plate that allowed simultaneous detection of the elemental spectra from mass 7-240.

Sample Preparation

Solid samples were prepared by mixing a 0.1 g sample with 0.1 g of ultrapure graphite in an agate mortar, adding the internal element standard along with a few drops of redistilled alcohol, and then evaporating the alcohol and water from the mix with an infrared lamp.

Liquid samples were prepared by mixing a 25-ml aliquot of sample with 0.2 g of ultrapure graphite in an agate mortar, adding the internal element standard along with a few drops of redistilled alcohol, and evaporating the alcohol and water from the mix with an infrared lamp.

The resulting mix was then compacted into polyethylene slugs and inserted into a metal die. Hydraulic pressure was applied to the die and slug forming a graphite electrode that was then mounted in a spark-source for analysis.(23)

When excessive amounts of organics were contained in any of the solid or the liquid samples, it was necessary to ash the sample thermally in a quartz container at 350°C with an appropriate amount of ultrapure graphite and the internal element standard. This procedure was necessary to eliminate interfering hydrocarbons for easier analysis and data interpretation.

Spark-Source Analysis

To exemplify the procedures used, an example of trace element determination will be presented. In general for a solid sample, calculated detection limits for each element were presupposed on several points: (1) a 0.1 g solid sample; (2) 0.1 g of ultrapure graphite used for spark-source electrode; (3) internal element standard added at 10 μg/ml sample; (4) a total of 210 nanocoulombs (nC) to be taken from side of the electrode in decreasing exposure on the plate: 100, 60, 30, 10, 6, 3, 1, 0.06, 0.01, 0.006 and 0.001 nC. This series of exposure covered the ppm concentration range for most trace elements.

Elemental detection limits of ~0.1-0.5 ppm were met and exceeded in most cases on solid samples. For a liquid sample calculated detection limits for each element were presupposed on several points: (1) a 25 ml sample; (2) 0.2 g of ultrapure graphite used for spark-source electrode; (3) internal standards added at 10 μg/ml sample; (4) a total of 210 nC to be taken from each set of electrodes in the same manner of decreasing exposure as for solid samples. This series of exposures covered the ppb concentration range for most trace elements. Elemental detection limits of ~1-2 ppb were met and exceeded in most cases on a liquid sample.

The calculation of concentrations was based on relative sensitivity factors determined from the elemental spike, which was indium. Detection limits were estimated by a "just disappearing line" technique. An example of this method is described here for barium.

The element barium has seven naturally occurring isotopes at mass-to-charge (m/e) of 130, 132, 134, 135, 136, 137 and 138. The relative isotope abundances are 0.108%, 0.119%, 2.44%, 6.58%, 7.87%, 11.41% and 71.05%, respectively. Detection limits for barium which exemplify the calculations also for other elements were as follows:

$$\text{sp} = \frac{\text{Conc. Std. x Just Detectable Exposure}}{\text{Longest Exposure}}$$

where

sp = photographic plate sensitivity, i.e., the relative concentration in ppm weight of any isotope that is "just detectable" on the longest exposure

When indium is used in a concentration of 10 μg per 0.1 g of solid sample the indium 115 isotope "just disappears" on the 0.1 nC line. Therefore, assume:

0.1 g solid sample
10 μg indium internal standard
indium 115 isotope 96.67% natural abundance
indium 113 isotope 4.24% natural abundance

$$\text{sp} = \frac{0.1\ \text{nC}}{100\ \text{nC}} \times \frac{10\ \mu\text{g}}{0.1\ \text{g}} \times 0.9567$$

Concentration of the impurity element can then be calculated.

$$\text{Conc.} = \text{sp} \times \frac{\text{longest exposure}}{\text{mass of std. isotope}} \times \frac{\text{mass element}}{\text{just detectable exposure}} \times \text{isotopic factor} \times \text{relative sensitivity factor}$$

The relative sensitivity factors (RSS) were used which are average sensitivity factors for a variety of matrices.

For barium then, a detection limit was calculated if the m/e 138 isotope of barium "just disappeared" on the 100 nC exposure as follows:

$$\text{Conc. barium}\ \mu\text{g/g} = 9.9 \times 10^{-2} \times \frac{100}{115} \times \frac{138}{100} \times 1.4 \times 1\ \text{RSF}$$

or

Conc. barium μg/g = 1.6×10^{-1} μg/g or this can be expressed as 0.16 μg/g (0.16 ppm).

Similar calculations were used for each of the trace elements occurring in the energy-related waste and effluent samples to obtain calculated detection limits.

Plate Interpretation(24)

Photoplate interpretation was carried out using the "just disappearing" line method. Photoplate detection allowed the simultaneous determination of all ion spectra and provided a reproducibility of response of ±3-5%.

Precision and Accuracy

Accuracy was related to ability to determine precisely elemental values both in a standard and in a given sample. The degree of certainty of analysis was then related to precision and thus to accuracy. Pulson, Elvesier and Keller(25) determined that isotope dilution spark-source mass spectrometry can be good as 3%, but ranges from 3-10% at 95% confidence limit. Total overall precision when the densitometer method is used (condensed from a variety of literature references) is ~3-20% using a photoplate recording device.(26-29) Precision in applying the "just disappearing line" technique was normally ±100% at a 1 ppm concentration level. Accuracies were related to the external standard.

ORGANIC COMPOUNDS

Sample Preparation

Volatiles--

Volatile organic compounds were recovered from water and tar samples using previously developed methods.(30-37) An aliquot of the water (3-100 ml) or tar (5 μℓ) sample was appropriately diluted with deionized-distilled water to a constant volume (100 ml), placed in a glass vessel, and the volatiles purged with an ultra-pure stream of helium gas (Fig. 2). The helium stream passed through a short glass condenser to eliminate the bulk of water vapor. The volatile compounds were trapped in a glass cartridge containing Tenax GC sorbent (2,6-diphenyl-p-phenylene oxide, Applied Science Lab., State College, PA, 35/60 mesh).(31,32,36,37) The preparation and conditioning of the Tenax GC sampling cartridge (bed dimension of 1.5 cm x 8 cm) has been previously reported.(38,39) Volatiles were purged by heating the liquid sample to 40-60°C at a flow of 25 ml/min of helium for 90 min (Fig 2). Previous research at RTI had indicated that these conditions were necessary for quantitative recovery of organic compounds up to a volatility, molecular weight and solubility similar to naphthalene and C_{14} aliphatic hydrocarbons for non-polar compounds and of compounds containing heteroatoms (oxygen, nitrogen and sulfur) without active hydrogens up to a molecular weight of ~150 with an appreciable volatility (semi-polar group). The highly polar compounds containing active hydrogens (e.g., alcohols, acids and amines) could not be quantitated by the procedure; however, they were analyzed after solvent extraction and derivatization.

The quantitative trapping and retainment of organic vapors on Tenax GC had been previously determined in our laboratories by using a backup cartridge to ensure that the flow rate and purging time used did not exceed the breakthrough volume of the sorbent for each organic compound purged. Also, after 90 min of He purging, the Tenax GC cartridge was replaced with a virgin one, and the liquid sample was purged for an additional 90 min. Less than 10% additional volatiles were recovered during the second 90 min.

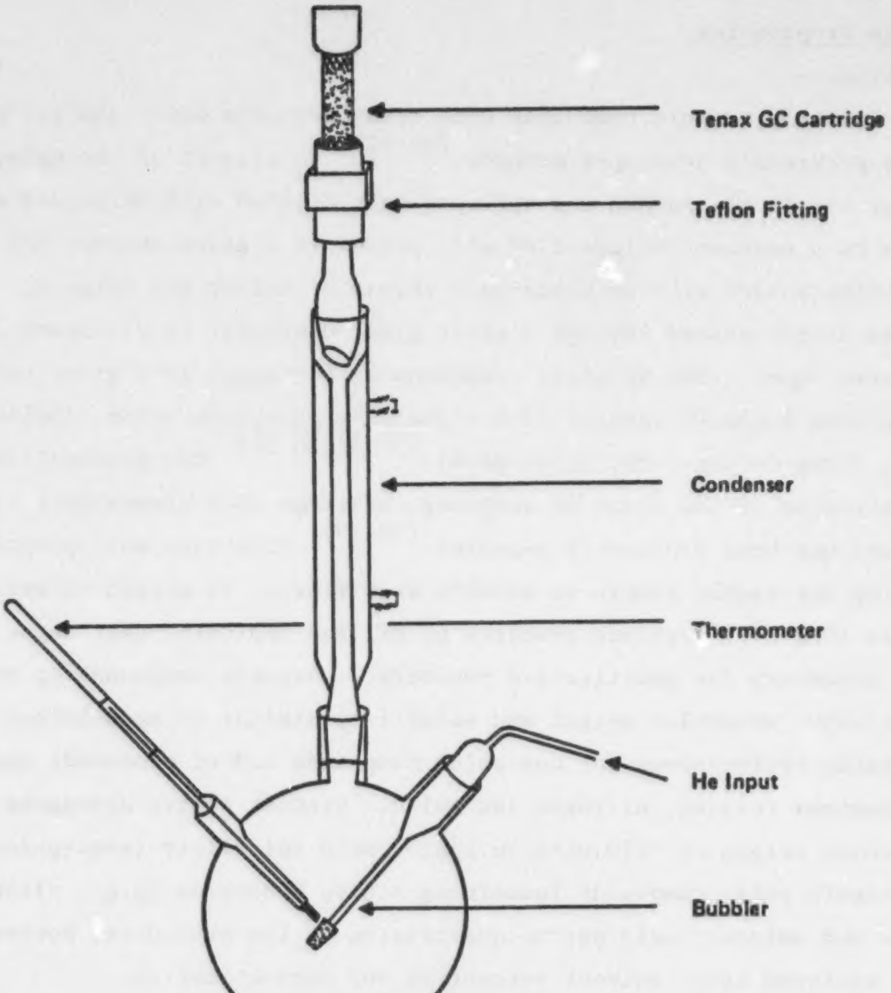

Tenax GC Cartridge
Teflon Fitting
Condenser
Thermometer
He Input
Bubbler

Figure 2. Apparatus for VOA purge

The Tenax GC cartridges containing volatile organics were analyzed by thermal desorption techniques using an inlet-manifold system previously developed at RTI.(36-38)

In cases where excessive foaming occurred, the lowest temperature (40°C) allowable for quantitative recovery was used in combination with vigorous stirring. For this reason a round bottom flask as depicted in Fig. 2 was used.

During the course of the program, a dehydration step was included to remove excess water from the Tenax cartridge prior to instrumental analysis. Tenax cartridges were stored over 1 g $CaSO_4$ for 2 hr in Kimax® culture tubes immediately after purging and then stored as previously described. Comparison of replicate cartridges with and without a drying step indicated no loss of organic volatiles.

SAMPLE PREPARATION

Semi-volatile organic compounds normally not recovered by the above procedure were extracted from water (100 ml) and tar (5-10 μg) by transferring a fresh sample to a separatory funnel equipped with a teflon stopcock and partitioning with Freon-TF®. The fractionation scheme is shown in Fig. 3. The pH of the aqueous solution was adjusted to >11 and <4 with 1N NaOH and 1N HCl, respectively, for the extraction of basic and acidic compounds. Prior to its use, Freon-TF® was purified by florisil column chromatography. Organic solvent blanks were simultaneously processed.

The combined organic solvent extracts (3) were concentrated in a Kuderna-Danish apparatus to ~300 μℓ and the final volume was measured to the nearest 10 μℓ and the concentration of substances was expressed in ppb or ppm in the original liquid sample.

Aqueous Process Effluents

Neutral Fraction--

The fraction containing neutral compounds derived from extraction of the Freon-TF® phase with aqueous acid was concentrated for analysis. The organic layers were combined and evaporated in a Kuderna-Danish apparatus. The concentrate was submitted directly to glc/ms/comp analysis.

Basic Fraction--

The aqueous acid fraction remaining after the removal of neutrals was adjusted to pH 12 with 5N NaOH and extracted with four 100-ml portions of

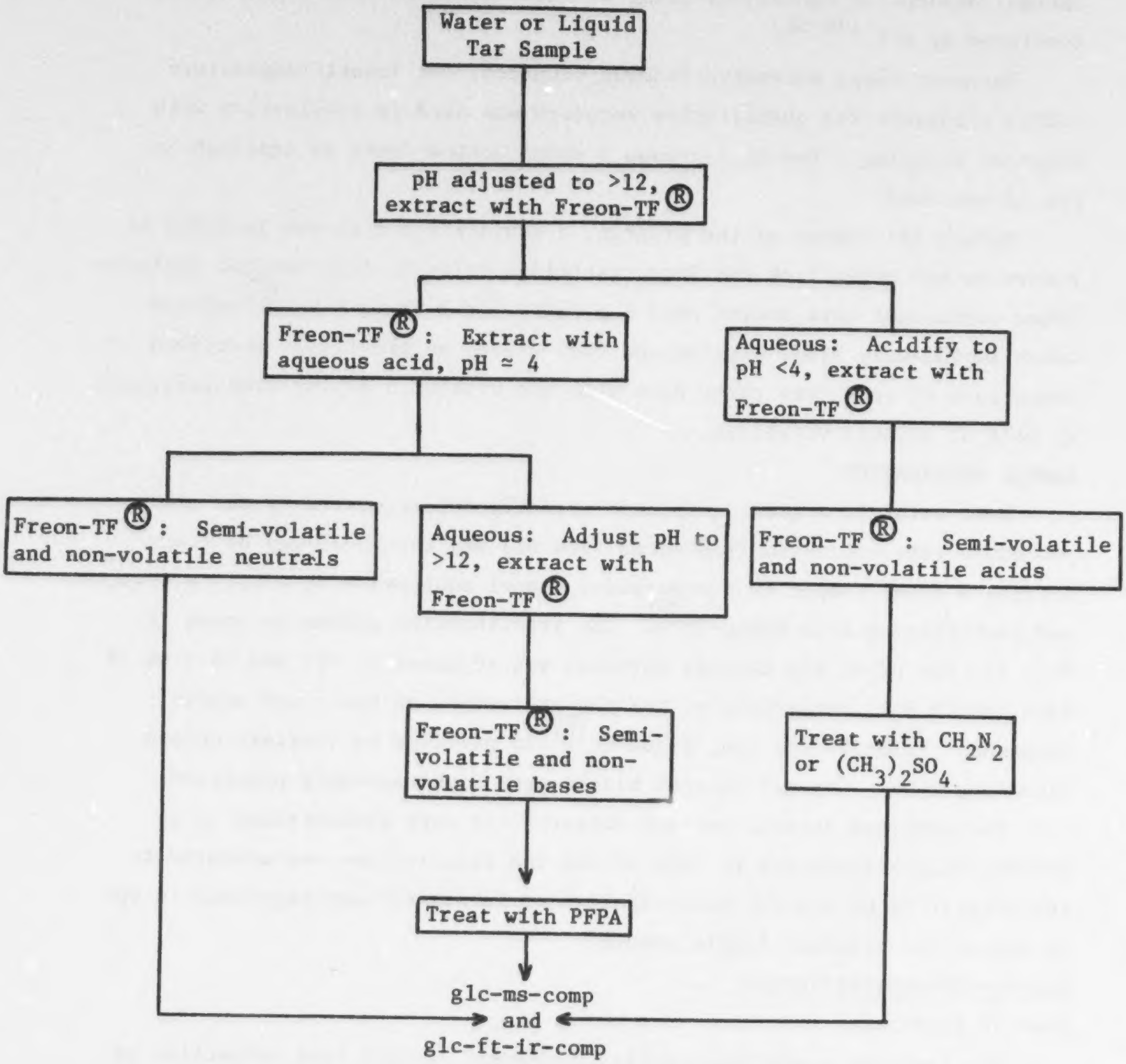

Water or Liquid Tar Sample
pH adjusted to >12, extract with Freon-TF®
Freon-TF®: Extract with aqueous acid, pH ≃ 4
Aqueous: Acidify to pH <4, extract with Freon-TF®
Freon-TF®: Semi-volatile and non-volatile neutrals
Aqueous: Adjust pH to >12, extract with Freon-TF®
Freon-TF®: Semi-volatile and non-volatile acids
Freon-TF®: Semi-volatile and non-volatile bases
Treat with CH_2N_2 or $(CH_3)_2SO_4$
Treat with PFPA
glc-ms-comp and glc-ft-ir-comp

Figure 3. Schematic for recovery and analysis of semi-volatile organics from water or liquid tar samples.

organic solvent. The organic phases were combined and evaporated in a Kuderna-Danish apparatus. The Kuderna-Danish reservoir was rinsed and the concentrate and rinsings combined and further evaporated under a slow stream of N_2 to 300 μℓ. The concentrate containing basic compounds were derivatized by treatment with perfluoropropionic anhydride (100 μℓ). The mixture was heated to 35-45°C for 1 hr and neutralized with a few drops of 5% $NaHCO_3$. The lower organic layer was transferred to a graduated Reacti-vial® concentrated to 300 μℓ under a slow stream of nitrogen and submitted to instrumental analysis.

Acidic Fraction--

The original alkaline aqueous layer was adjusted to pH 4 with 1N HCl and extracted with four 100-ml portions of organic solvent. The organic layers were combined and concentrated to 2 ml. The apparatus was rinsed and the rinsings were combined with the original concentrate and further evaporated under slow stream of nitrogen to 300 μℓ. The concentrate was treated with diazomethane to methylate the acidic components.(40) This procedure satisfactorily converted the carboxylic acids; however, the phenols were chromatographed as the parent compounds.

Tar/Oils and Solid Samples

The organic compounds in oil or tar were fractionated by dissolving 5-10 μℓ of sample in 100 ml of Freon-TF®. The Freon-TF® layer was then extracted with an equal volume of 1N HCl to remove organic bases. The aqueous acid layer was then adjusted to pH 11 with 5N NaOH and the organics recovered by multiple organic solvent extractions. The original Freon-TF® fraction was then partitioned with base to separate neutral and acidic compounds. Derivatization of the acidic and basic fractions were carried out as described below.

ANALYSIS BY GLC/MS/COMP

Volatiles

Recovery of Volatile Organics Collected on Tenax GC Cartridge Samplers--

The inlet-manifold (Fig. 4) for recovering volatile organics trapped on Tenax GC cartridges was previously developed under a research program at RTI (EPA Contract No. 68-02-1228) and was used in this program.(36-39) The design and performance of the inlet-manifold system have been previously discussed.(36-39)

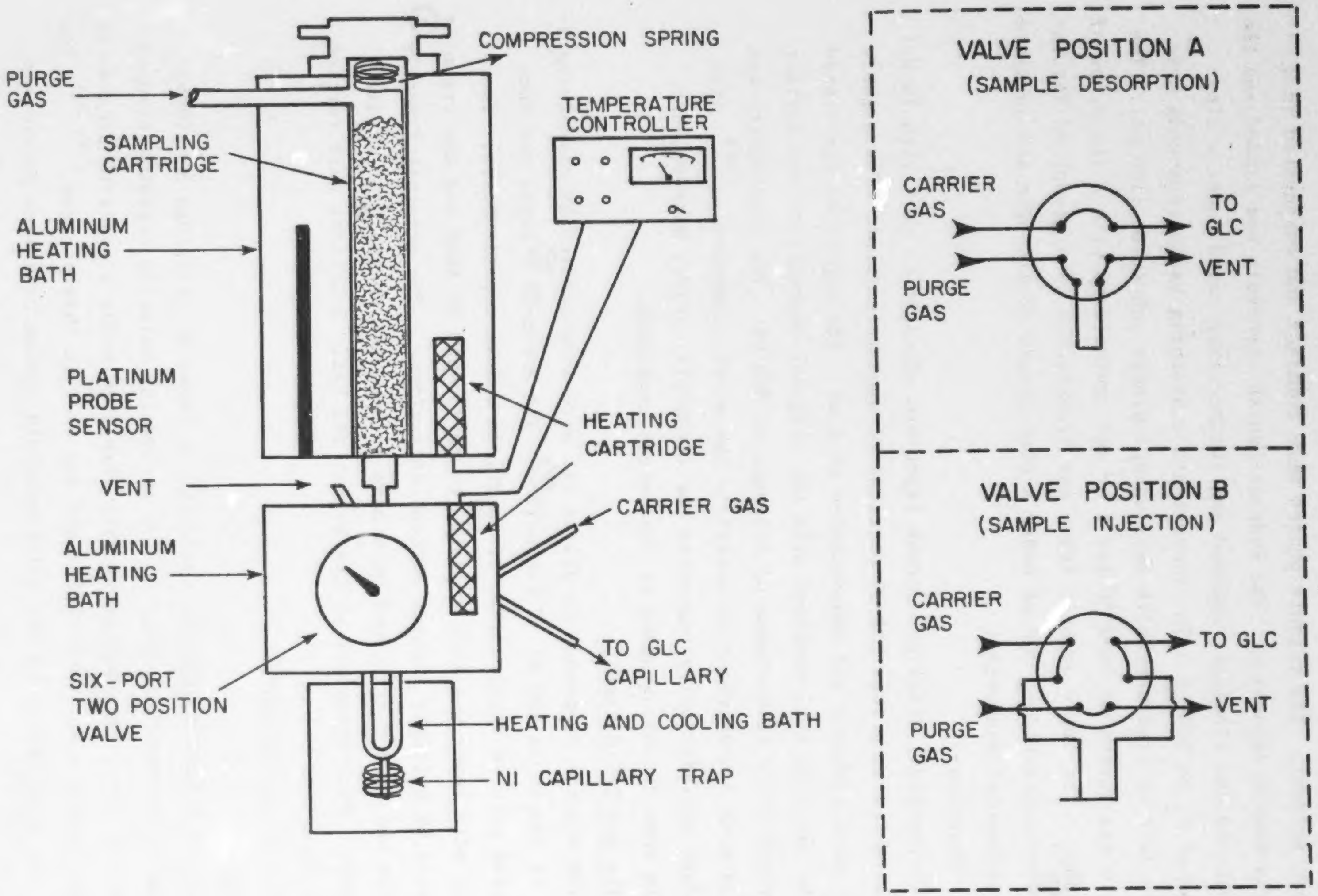

PURGE GAS
SAMPLING CARTRIDGE
ALUMINUM HEATING BATH
PLATINUM PROBE SENSOR
VENT
ALUMINUM HEATING BATH
SIX-PORT TWO POSITION VALVE
COMPRESSION SPRING
TEMPERATURE CONTROLLER
HEATING CARTRIDGE
CARRIER GAS
TO GLC CAPILLARY
HEATING AND COOLING BATH
NI CAPILLARY TRAP
VALVE POSITION A
(SAMPLE DESORPTION)
CARRIER GAS
PURGE GAS
TO GLC
VENT
VALVE POSITION B
(SAMPLE INJECTION)
CARRIER GAS
PURGE GAS
TO GLC
VENT

Figure 4. Thermal desorption inlet-manifold

In a typical thermal desorption cycle, a Tenax GC cartridge was placed in the preheated chamber (~270°C) and the helium gas was passed through the cartridge (~20 ml/min) to purge the vapors into the liquid nitrogen cooled Ni capillary trap. These conditions constitute the valve position "A" (Fig. 4). After the thermal desorption step was completed (~4 min), the six-port valve was rotated to position "B" (Fig. 4) and the temperature on the capillary loop was rapidly raised whereupon the carrier gas carried the vapors onto a high resolution glass capillary column (Support Coated Open Tubular, SCOT).

Gc/ms/comp Operating Parameters--

The desorbed vapors were subsequently resolved and mass cracking patterns were automatically and continuously obtained throughout the glc run with a Varian MAT CH-7 mass spectrometer/620L computer system. Figure 5 depicts a schematic of this system. The operating parameters are given in Table 5. The SCOT column, which was prepared by previously described techniques in this laboratory,(38,39) was coated with OV-101 stationary phase. The elution order for over 200 compounds was established using authentic materials.

Typically the mass spectrometer was set to operate in the repetitive scanning mode. In this mode, the magnet was automatically scanned exponentially upward from a preset low to high mass value. Although the scan range could be varied depending on the particular sample, typically the range was from m/e 28 to m/e 400. The scan cycle was completed in approximately 3 sec. At this time the instrument automatically reset itself to the low mass position in preparation for the next scan and the information was accumulated by an on-line 620/L computer onto magnetic tapes. The reset period required approximately 3 sec, thus a continuous scan cycle of <6 sec was maintained.

Prior to running unknown samples, the system was calibrated by introducing a standard substance such as perfluorokerosene into the instrument and determining the time of appearance of the known standard peak in relation to the scanning magnetic field. The calibration curve was stored in the 620/L computer memory.

With the magnet continuously scanning, the sample was injected and automatic data acquisition was initiated. As each spectrum was acquired by

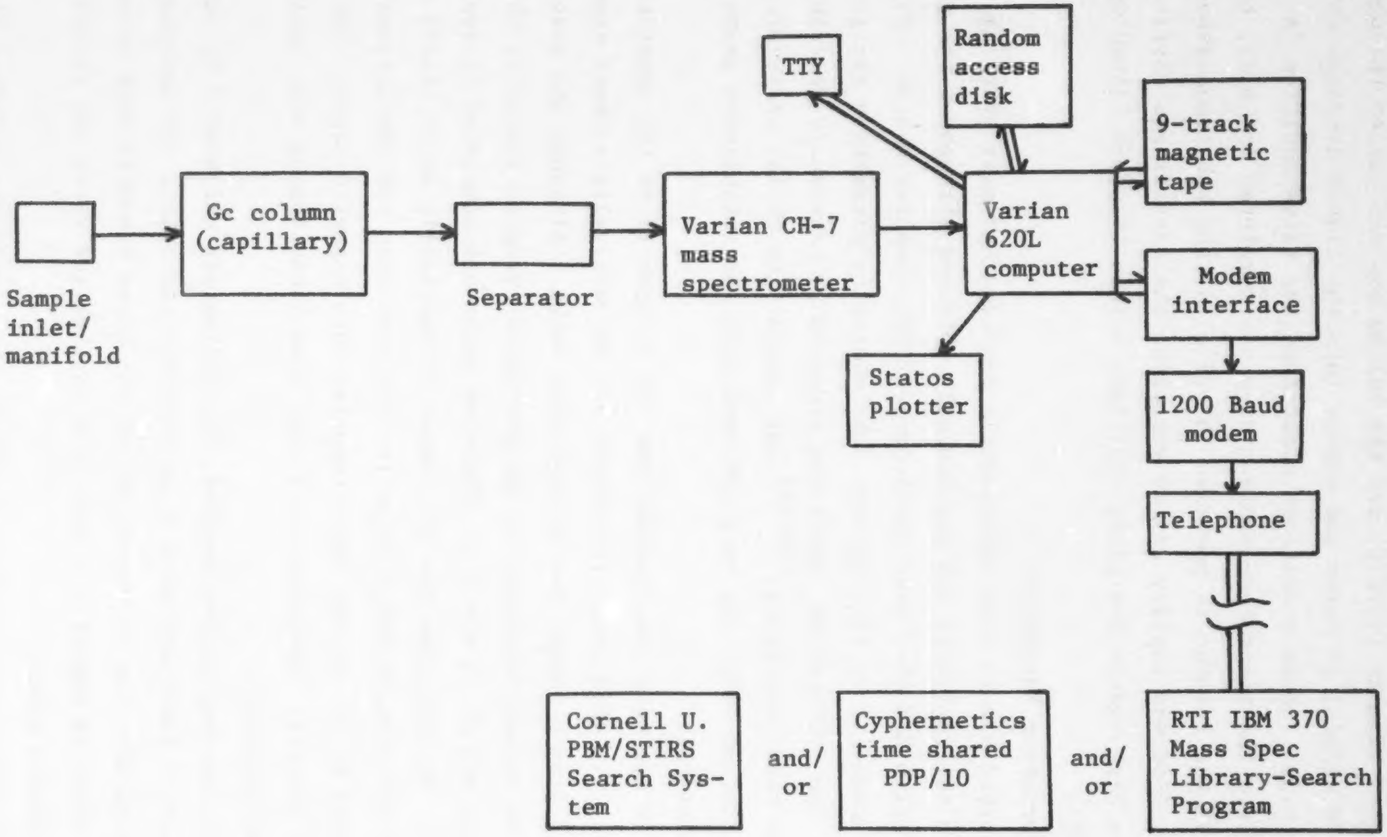

Sample
inlet/
manifold
Gc column
(capillary)
Separator
Varian CH-7
mass
spectrometer
TTY
Random
access
disk
Varian
620L
computer
Statos
plotter
9-track
magnetic
tape
Modem
interface
1200 Baud
modem
Telephone
Cornell U.
PBM/STIRS
Search Sys-
tem
and/
or
Cyphernetics
time shared
PDP/10
and/
or
RTI IBM 370
Mass Spec
Library-Search
Program

Figure 5. Schematic diagram of gc-ms computer system and library search systems

Table 5. OPERATING PARAMETERS FOR GLC-MS-COMP SYSTEM

Parameter	Setting
Inlet-manifold	
desorption chamber	270°C
valve	220°C
capillary trap - minimum	-195°C
maximum	220°C
thermal desorption time	4 min
GLC	
100 m glass SCOT OV-101	20-240°C, 4/C° min
50 m glass SCOT Carbowax 20M	80-240°C
carrier (He) flow	~3 ml/min
transfer line to ms	240°C
MS	
scan range	m/e 20 → 300
scan rate, automatic-cyclic	1 sec/decade
filament current	300 μA
multiplier	6.0
ion source vacuum	$\sim 4 \times 10^{-6}$ torr

the computer, each peak which exceeded a preset threshold was recognized and reduced to centroid time and peak intensity. This information was stored in the computer core while the scan was in progress. In addition approximately 30 TIC values and an equal number of Hall probe signals were stored in core as they were acquired. During the 3-sec period between scans, this spectral information along with the spectrum number was written sequentially on magnetic tape and the computer was reset for the acquisition of the next spectrum.

This procedure continued until the entire gc run was completed. By this time there were from 300-1,000 spectra which were then subsequently processed. Depending on circumstances, the data were either processed immediately or additional samples were run, stored on magnetic tape and the results examined at a later time.

The mass spectral data were processed in the following manner. First the original spectra were scanned and the TIC information was extracted. Then the TIC intensities were plotted against spectrum number on a Statos 3185 recorder. The information was generally indicative of whether the run was suitable for further processing since it gave some idea of the number of knowns in the sample and the resolution obtained using the particular glc column conditions.

The next stage of the processing involved mass conversion of the spectral peak times to peak masses, which was done directly via the Dual Disk System. The mass conversion was accomplished by use of the calibration table obtained previously. Normally one set of calibration data was sufficient for an entire day's data processing since the characteristics of the Hall probe for the variation of calibration was <0.2 atomic mass units/day. Nevertheless the calibration table was checked to make sure that variation in the atomic mass units assignment did not occur. A typical time required for this conversion process for 1,000 spectra was approximately 30 min.

After the spectra were obtained in mass converted form, processing proceeded either manually or by computer. In the manual mode, the full spectra of scans from the gc run were recorded on a Statos 3185 printer-plotter. The TIC information available at this time was most useful for deciding which spectra were to be analyzed. In most cases, the chromatographic run was extremely rich and all the spectra needed to be outputt and individually interpreted.

Semi-Volatiles

The semi-volatile organic compounds (neutral, methylated acids and derivatized base fractions) were analyzed by high resolution glass capillary column gc/ms/comp techniques using a splitless injection method. The previously described inlet-manifold was used for introducing the semi-volatile compounds in the following manner. A 3-5 μℓ aliquot was applied to glass wool (0.5 cm x 1.5 cm in length) in a glass cartridge. After the solvent had evaporated (approximately 3 min), the desorption through the inlet-manifold and injection into the high resolution column was essentially the same as described for volatile organics. For the analysis of semi-volatile organic compounds, a 50-m glass SCOT column coated with Carbowax 20 M was used for effecting the resolution of the components in the mixture (Table 5).

ANALYSIS BY GAS CHROMATOGRAPHIC FOURIER TRANSFORM INFRARED SPECTOSCOPY COMPUTER TECHNIQUES

In general, methods of organic compound identification rely on the empirical correlation between molecular properties and the observed data. Ambiguity in substance identification can be expected and confirmation by two or more independent analytical methods is preferable. The unique structural information on the molecule contained in the infra-red spectrum when combined with those derived from other analytical methods greatly reduced the uncertainties in the identification of trace quantities of substances.

Although the primary technique employed for trace organic characterization of energy-related effluents in this program was high resolution gc/ms/comp, we also used gas chromatography/Fourier transform infrared spectroscopy/computer (gc/ftir/comp) techniques for characterization of semi-volatile organic compounds. The application of the gc/ftir/comp to analysis of the organics in energy samples was confined to a few samples, in particular, the semi-volatile components of the acid fraction.

DATA INTERPRETATION

Identification of resolved components was achieved by comparing the mass cracking pattern of the unknown to an eight major peak index of mass spectra.(41) Individual difficult unknowns were submitted to the Cornell University STIRS and PBM systems and/or the EPA MSSS System (Cyphernetics) for identification. When available, authentic compounds of the tentatively identified components were obtained and chromatographed under identical conditions on the OV-101 or Carbowax 20 M glass capillary column. The elution time and temperature for the authentic compounds was compared to the unknown in order to establish further the identity of the component. Particular note was made of the comparison of the boiling point of the tentatively identified compound with the elution temperature and the order of elution of other constituents in the same homologous series since the OV-101 SCOT capillary column separates primarily on the basis of boiling point.

The identity of the components in energy samples was assigned on a graded scale. Positive identification was assigned for those compounds for which the observed spectra matched library spectra and/or indexes of tabulated spectra and the elution time and temperature corresponded with that of an authentic compound. In many cases where the isomeric form could not be distinguished, the name of the compound as an isomer was indicated. In many cases, only an empirical formula could be assigned since the mass cracking patterns of isomers were very similar and the retention index could not be determined for all of the isomers since all the authentic compounds were not available. In some cases, a tentative identification was assigned when the mass cracking pattern yielded a "similar" match, and no retention index was available for that compound.

QUANTIFICATION OF VOLATILES AND SEMI-VOLATILES

The volatile and semi-volatile compounds were quantitated by glc/ms/comp utilizing the total ion current monitor and, when necessary, mass fragmentography. In order to eliminate the need to obtain complete calibration curves for each compound for which quantititative information was desired, we used the method of relative molar response (RMR) factors. Successful use of this method required information on the exact amount of reference standard added and the relationship of the RMR for the unknown to the RMR of the standard. The method of calculation was as follows:

$$(1) \quad RMR_{unknown/standard} = \frac{A_{unk}/Moles_{unk}}{A_{std}/Moles_{std}}$$

A = peak area, determined by integration or triangulation.

The value of RMR is determined from at least three independent analyses.

$$(2) \quad RMR_{unk/std} = \frac{A_{unk}/g_{unk}/GMW_{unk}}{A_{std}/g_{std}/GMW_{std}}$$

A = peak area, as above
g = number of grams present
GMW = gram molecular weight

Thus, in the sample analyzed:

$$(3) \quad g_{unk} = \frac{A_{unk} \cdot GMS_{unk} \cdot g_{std}}{A_{std} \cdot GMW_{std} \cdot RMR_{unk/std}}$$

The reference standards were added after the volatile organics were trapped on a Tenax GC sampling cartridge but prior to thermal desorption or were added directly to the Kuderna-Danish concentrate. For the quantification of volatile organic compounds, the two reference standards were hexafluorobenzene and perfluorotoluene (200 ng each). These compounds were observed in previous research to elute from an OV-101 glass capillary column at a temperature and retention time which did not interfere with the analysis of unknown compounds in the samples. Used as the reference standard for quantification of semi-volatile organic compounds was d_5-nitrobenzene (200 ng).

The volume of the sample used for purging volatiles or the extraction of semi-volatile compounds was accurately measured (±1%) prior to processing. The concentration was calculated in ppm or ppb. The major advantage of this technique was that once the reference standard had been added to a sample containing a series of unknown compounds, the quantity of the unknowns could be determined after their identities had been established. The relative molar response ratio was calculated by using an authenic standard of that compound or an analog. A disadvantage of this approach is that a wide range of volatility of compounds was observed and the chromatographic separation occurred over a wide temperature range (20-240°C). The reproducibility (±50%) here is less than what can be achieved when an internal standard is used which has physical and chemical properties more closely resembling the compounds to be quantified. Because of the complexity of these samples, however, it was not feasible to utilize a large number of standards for the purpose of quantification. Nevertheless, as can be seen in the data, the reproducibility was in most cases well within a factor of two. Using this approach, it was also possible to obtain both qualitative and quantitative information on a single sample since it was possible to characterize the sample first and then return at a later time to the data stored on magnetic tape to determine the concentration of each of the constituents in the sample.

QUALITY CONTROL PROCEDURES

An analytical quality control and assurance program that applied to qualitative and quantitative analysis of trace organics was divided into five categories: (a) sample and data logging; (b) reagent and glassware control; (c) instrumentation control; (d) supporting experiments; and (e) data evaluation. The quality control associated with sampling procedures and data logging is given in Section 6.

Reagents and Glassware

In order to minimize the introduction of contamination from the materials used in the purification procedures, we used a reagent and glassware control that incorporated blanks. High quality commercial reagents and solvents are available, but the quality can be somewhat variable and unpredictable. The Freon-TF® which was used for extraction of semi-volatiles was purified by florisil column chromatography prior to its use and then concentrated by a factor of 100 to determine the potential contaminants. This procedure was repeated with each new lot of Freon-TF®. The deionized-distilled water was obtained by passing tap water through an ion exchange bed and a carbon adsorption cartridge to remove trace elements and organic constituents, respectively, prior to its distillation. For determining the background constituents during purging of volatile organics, the water which was used for the dilution of the liquid samples was independently assessed for background contamination by subjecting the water to the entire analytical procedure including gc/ms analysis. All glassware was cleaned with Isoclean, rinsed successively with deionized-distilled water, HCl, deionized water and then heated to 450°-500°C to insure the removal of all traces of organic compounds.

Instrumental Control

Instrumental control techniques were employed to insure that the total operating system was calibrated and in proper working order. This was performed by procedures which employ the use of a standard reference mixture and a set of reference criteria to evaluate the performance of the overall high resolution gc/ms/comp system. The standard reference mixture contained 12 compounds which represented non-polar, semi-polar and polar substances. This reference mixture was subjected to high resolution gc/ms/ comp analysis at the beginning of each working day. In this manner the performance of the high resolution gc column, the sensitivity of the mass spectrometer, the calibration of the mass spectrometer and the performance of the computer system was monitored by evaluating the results of the reference mixture.

Radiolabeled Recovery Studies

To determine the efficiency of recovery for the volatile and semi-volatile purification procedures, radiolabeled compounds were employed. Toluene[Ring-^{14}C, 4.0 μC/mM], benzene [^{14}C (U), 14.7 μC/mM], palmitic acid [^{14}C (U), 613 μC/mM], benzoic acid [7-^{14}C, 13.6 μC/mM] phenol [^{14}C (U), 10.7 μC/mM], acetone [2-^{14}C, 6.5 μC/mM], dimethylbenzanthracene-^{14}C, phenyl ethyl amine·HCl-^{14}C, and 3-amino-1,2,4-triazole were purchased from New England Corporation, Boston, MA. Acetonitrile [1-^{14}C, 14.9 μC/mM] and *n*-hexanoic acid [1-^{14}C, 58 μC/mM] were purchased from Amersham Searle, Corp. Plains, IL.

The radioisotopes were diluted in distilled deionized water to a final concentration of a few microcuries/milliliter. Energy samples spiked with individual radiolabeled compounds prior to sample purification, aliquots of the solid sorbent Tenax and liquid fractions from the liquid-liquid fractionation scheme were counted in a Packard Tricarb 3375 liquid scintillation spectrometer. To the fraction was added 15 ml of scintillation fluid and the sample was counted until a standard error of 2.5 was obtained. The scintillation fluid contained 18 g of Omnifluor, 1 ℓ of Triton-X and 2 ℓ of toluene. Observed radioactivity was corrected for quenching by the external standard ratio method and also evaluated by the addition of known quantities of radiolabeled compounds to each of the fractions to be counted. All counts were converted to disintegrations per minute.

The use of radiolabeled compounds allowed an assessment of the individual steps utilized for the recovery of the organic constituents as volatiles, and semi-volatile organic acids, bases and neutral compounds prior to instrumental analysis. Although all samples were not subjected to radiolabeled recovery studies, selected energy samples were processed which represented the various types of energy-related processes in order to assess the reliability of the purging and liquid-liquid extraction schemes.

SECTION 8

RESULTS AND DISCUSSION

METHODS OF ANALYSIS

Radiolabeled Recovery Studies

Volatiles--

The recovery of volatile organic compounds from aqueous solutions has been studied in several laboratories.(30-32,42) The technique as described in Section 7 employs an inert gas, helium, which is bubbled through the sample to transfer the volatile compounds from the aqueous phase to the gaseous phase and trap them on Tenax GC, a solid sorbent. The recovery of carbon-14 labeled acetone, acetonitrile, benzene and toluene from several aqueous samples from energy-related processes (in situ coal gasification) was determined. For compounds which are highly soluble in water, e.g., acetonitrile, the recovery by this method was found to be very low (~10%). The recovery of ^{14}C-labeled acetone was ~50%. On the other hand, the recovery of hydrocarbons, aromatics (benzene and toluene) and alkyl-aromatics was $\geq$ 80%. These observations are consistent with the reported data for recovery of volatile organics from sewage treatment effluents.(30)

In general, the purging of volatile organics from an aqueous medium utilizing an inert gas is quantitative for compounds with boiling points $\leq$210° and <2% solubility and for compounds with boiling points of <150° with a solubility <10% in water. Utilizing the percentage recoveries which were determined for ketones, aliphatic and aromatic hydrocarbons, thiophenes and aldehydes, the concentration was calculated for each specific sample component by correcting for the percentage recovery.

Semi-Volatiles--

The percentage recovery of selected radiolabeled compounds which were added to aqueous and tar samples from energy processes was determined for the liquid-liquid extraction method described in Section 7. The percentage recovery for a few selected neutral acidic and basic compounds was determined by their addition to several different energy samples. Table 6 presents the percentage recovery which was observed for the liquid-liquid extraction method employed. The percentage recovery presented in this table represents the average overall recovery observed prior to instrumental analysis. For toluene and dimethylbenzanthracene, essentially quantitative recovery was observed for the liquid-liquid extraction method and the Kuderna-Danish concentration steps. Quantitative recoveries for palmitic, hexanoic, and benzoic acids and phenol were also obtained. However, the highly water soluble butyric acid was not recovered from water by the liquid-liquid extraction method. It was concluded that, for quantification of acids utilizing this liquid-liquid extraction method, reliable data could be obtained for acids containing four or more methylene units.

Two bases were also subjected to the liquid-liquid extraction method to determine its efficiency. A recovery of ~68% was observed for phenyl ethyl amine in the basic fraction with only traces remaining in several other fractions. In contrast, the highly water soluble amine, 3-amino-1,2,4-triazole, could not be quantitatively extracted.

From these data, it was concluded that highly water soluble and/or low molecular weight compounds could not be recovered by this liquid-liquid extraction technique or retained in the receiver of the Kuderna-Danish apparatus. These data were used for calculating the quantities of the individual semi-volatile acids, bases, and neutral compounds in the energy samples.

Quantification by GC/MS/COMP Relative Molar Response (RMR) Factors

The RMR of several aliphatic and aromatic compounds based upon the total ion current monitor are presented in Table 7. For each compound, the RMR is presented as an average of five determinations along with their statistical variance and standard deviation. The RMR factors were calculated for the two external standards, perfluorobenzene and perfluorotoluene. As can be seen from these data, similar RMR's for the aliphatic hydrocarbons allow calculation of an "average RMR" for this chemical class. Thus, other compounds in the same chemical class for which authentic standards were not available could be quantified.

Many additional RMR's which are not presented in this table were determined and calculated, however, for the purpose of demonstrating this

Table 6. PERCENT RECOVERY OF SELECTED RADIOLABELED COMPOUNDS USING LIQUID/LIQUID EXTRACTION METHOD

	Fraction					
Radiolabeled Compound	Neutral	Acid	Base	H_2O/H^+[a]	H_2O/OH^-[b]	Total (Organic Phase)
Toluene	76 ± 9%	0.8 ± 0.4%	1.2 ± 0.6%	1.5 ± 1.0%	0%	79.5%
Dimethylbenzanthracene	83 ± 12%	3.0 ± 1.0%	0%	0%	0%	86.0%
Palmitic acid	31 ± 4%	80 ± 8%	0%	0%	0%	111.0%
Hexanoic acid	0%	75 ± 5%	0%	24 ± 3%	0%	75.0%
Benzoic acid	0%	54%	1.5%	45%	0%	55.5%
Butyric acid	0%	0%	0%	87 ± 13%	0%	0%
Phenol	0%	53 ± 3%	0%	46 ± 4%	0%	53%
Phenylethylamine	3 ± 2%	2 ± 1%	68 ± 7%	11 ± 3%	4 ± 2%	73.0%
3-Amino-1,2,4-triazole	0%	0%	0%	85 ± 14%	0%	0%

[a] Remaining after extraction of acidic solution.

[b] Remaining after extraction of basic solution.

Table 7 . EXAMPLES OF RELATIVE MOLAR RESPONSE (RMR) FACTORS FOR SEVERAL COMPOUNDS BASED UPON TOTAL ION CURRENT MONITOR

Compound	PFB[a]			PFT[a]		
	RMR	Var.[b]	S.D.[c]	RMR	Var.	S.D.
n-Heptane	1.39	0.150	0.39	1.66	0.080	0.29
n-Nonane	1.85	0.020	0.14	2.04	0.008	0.09
n-Undecane	1.71	0.048	0.22	1.94	0.016	0.12
n-Tridecane	1.31	0.130	0.36	1.44	0.110	0.34
1-Heptene	1.84	0.001	0.04	2.01	0.001	0.04
Di-*n*-butyl ether	5.90	0.300	0.55	6.40	0.130	0.36
2-Pentanone	2.84	0.260	0.41	2.94	0.060	0.240
2-Ethylfuran	2.59	0.230	0.48	2.68	0.100	0.320
Tetrahydronaphthalene	1.98	-	-	1.72	-	-
4-Vinyl-1-cyclohexene	1.59	0.040	0.22	1.84	0.010	0.10
Cyclohexene oxide	1.28	0.020	0.13	1.32	0.030	0.17
Toluene	2.38	0.020	0.15	2.48	0.110	0.33
Cumene	1.56	0.050	0.22	1.76	0.026	0.16
1,3,5-Trimethylbenzene	1.48	0.050	0.22	1.63	0.037	0.19
1,2,4-Trimethylbenzene	1.47	0.025	0.16	1.47	0.006	0.08
1,2,3-Trimethylbenzene	1.26	0.040	0.19	1.45	0.013	0.11
Phenylacetylene	1.25	0.001	0.03	1.45	0.010	0.12
Naphthalene	1.34	-	-	1.53	-	-
o-Xylene	2.90	0.170	0.42	2.33	0.200	0.41
Anisole	1.77	0.290	0.54	2.14	0.040	0.20
Acetophenone	1.58	0.040	0.20	1.79	0.007	0.08
2-Methylbenzofuran	1.46	0.003	0.06	1.32	0.030	0.18
α-Methylstyrene	1.88	0.001	0.01	2.04	0.004	0.06
Indan	1.54	0.024	0.16	1.76	0.027	0.16
m-Tolualdehyde	1.56	0.020	0.15	1.54	0.003	0.06
o-Ethylaniline	1.62	0.170	0.41	1.28	0.060	0.25

[a] PFB = perfluorobenzene, PFT = perfluorotoluene which were external standards.

[b] Var. = statistical variance.

[c] S.D. = standard deviation.

approach, these RMR's were selected for reporting. The RMR factors for several other compounds representing ketones, aldehydes, thiophenes, ethers, amines, anilines, acids, etc. were determined for those compounds which were commercially available and an "average RMR" value for each chemical class was used for estimating the concentrations of compounds appearing in the energy samples for which authentic standards were not available.

Table 8 presents selected examples of RMR factors for several compounds based upon fragment ions. The RMR factors were determined for two ions and utilizing mass fragmentography, the concentration of each compound in the unknown sample was determined. In a similar manner to the RMR calculated based upon the total ion current monitor, the RMR factors for selected fragment ions were determined for those authentic compounds which were commercially available and in those cases where authentic compounds were not available, an "average RMR" value was calculated for each homologous series. The use of mass fragmentography was necessary when inadequate resolution was observed in the total ion current monitor.

Table 8. EXAMPLES OF RELATIVE MOLAR RESPONSE FACTORS FOR SEVERAL COMPOUNDS BASED UPON SELECTED FRAGMENT IONS[a]

Compound	MW	1st Ion		2nd Ion	
		m/e (I)	RMR	m/e (I)	RMR
Toluene	92	91 (100)	2.37	64 (13)	0.66
o-Xylene	106	105 (27)	3.46	51 (10)	0.39
Anisole	108	108 (100)	1.19	65 (76)	1.30
Acetophenone	120	105 (100)	1.97	120 (29)	1.27
Naphthalene	128	128 (100)	1.92	51 (12)	0.18
2-Ethylfuran	96	81 (100)	2.35	-	-
2-Pentanone	86	43 (100)	1.98	57 (26)	0.14

[a] RMR values were calculated relative to m/e 186 (100) for the external standard, hexafluorobenzene.

Mass Fragmentography

The technique of mass fragmentography was utilized for the quantification of volatile and semi-volatile organics when inadequate resolution existed for the total ion current monitor. The use of ion chromatograms permitted the attainment of additional specificity (and better resolution) for the individual components in each of the samples. Even though high resolution glass capillary columns (SCOT's) were used for effecting the resolution of the components in each mixture, the separation efficiency of the capillaries was inadequate for obtaining baseline resolution for every constituent in the sample. Since it was impractical to utilize very high resolution capillaries, *e.g.* wall-coated open tubular (capacity too low) or very long SCOT capillaries, we chose the mass fragmentographic technique to obtain sufficient resolution for quantification of the individual species.

Figures 6-12 depict mass fragmentograms for several selected ions for the volatile organics in product water (-13L) from an *in situ* coal gasification experiment. In Fig. 6 peaks labeled 1(m/e 67), 2 and 3 (m/e 114), 4 (m/e 71) and 5 (m/e 186) represent the compounds pyrrole, *n*-octane, 2-heptanone and perfluorobenzene, respectively. Figure 7 presents the ion chromatograms for m/e 106 and 104 for the same sample. Where peaks 1-3 represent ethylbenzene, *p*- and *o*-xylene, respectively. Figure 8 represents ion chromatograms for m/e 121, 94, 95 and 120. Peaks 1-7 are isopropylbenzene, *n*-propylbenzene, *m*-,*p*-, and *o*-ethylbenzene; and 1,2,4-and 1,2,3-trimethylbenzenes, respectively. Figure 9 presents the ion chromatogram for m/e 85 which represents aliphatic hydrocarbons. Ion chromatograms for m/e 186 and 105 are given in Fig. 10 and the peaks 1-3 represent the xylenes and ethylbenzenes. Figure 11 presents the ion chromatograms for m/e 186 and 131 and the peaks 1-5 represent methylbenzofuran and several dimethylindans. Ion chromatograms for m/e 186, 156, 152 are in Fig. 12 and the peaks 1-6 are ethylnaphthalene and several dimethylnaphthalene isomers. Additional ion chromatograms were obtained for this sample which allowed the quantitation of essentially all of the components that were identified in the sample.

This approach was used throughout the research program for the quantification of organic volatile and semi-volatile compounds in energy samples.

Qualitative Analysis by GC/FTIR/COMP

Samples of the acid fraction from product water obtained during *in situ* coal gasification were analyzed by gc/ftir/comp to confirm and supplement identifications using gc/ms/comp. Samples were previously extracted

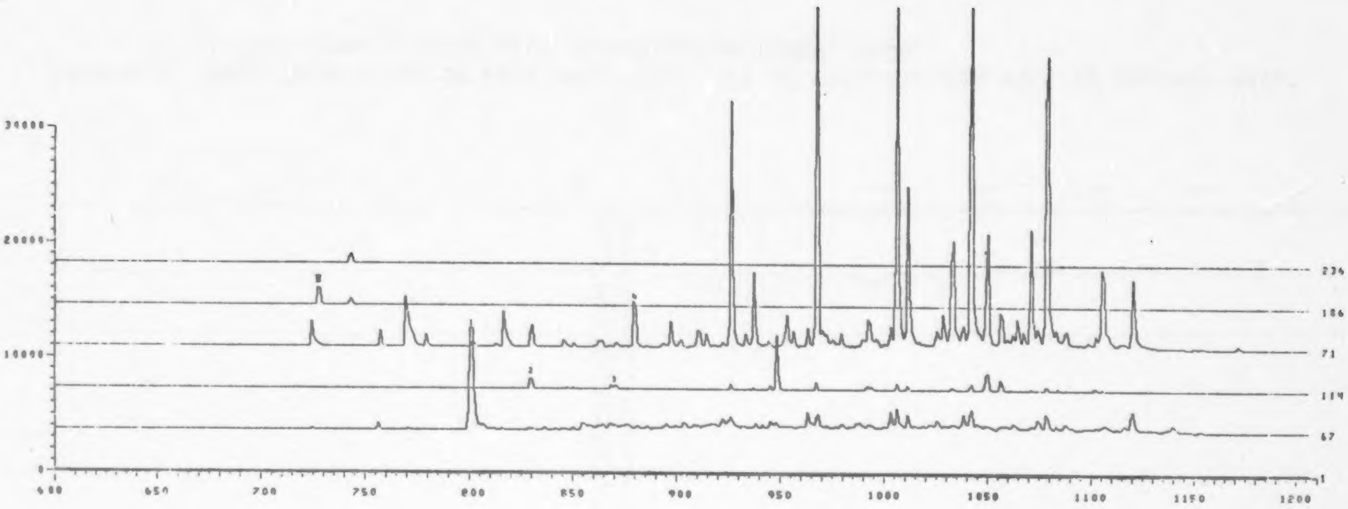


Figure 6. Mass fragmentogram (m/e 236, 186, 71, 114, 67) of volatile organics in product water (-13L) from in situ coal gasification (LERC, ERDA).

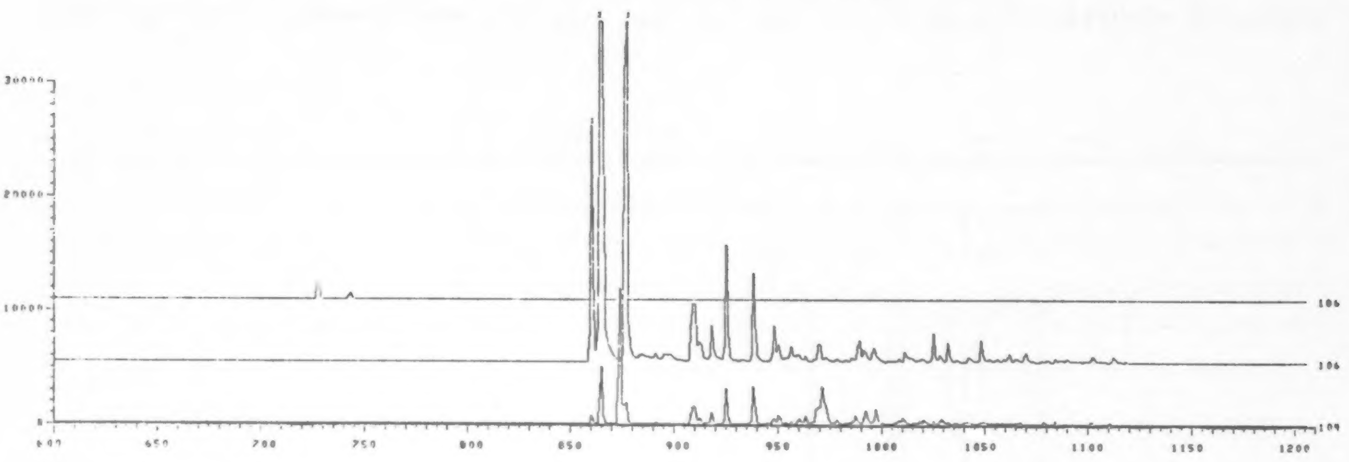


Figure 7. Mass fragmentogram (m/e 186, 106, 107) of volatile organics in product water (-13L) from in situ coal gasification (LERC, ERDA).

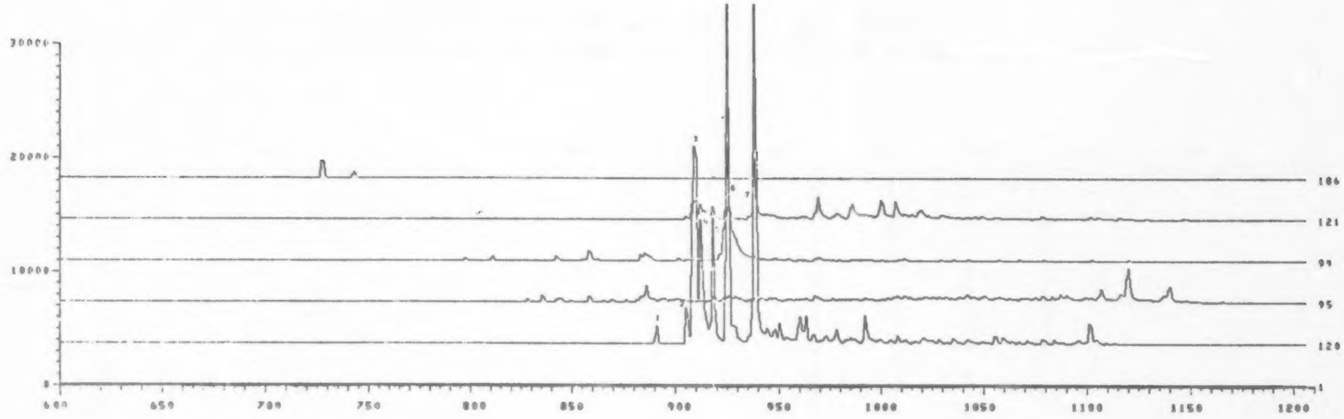


Figure 8. Mass fragmentograms (m/e 186, 121, 94, 95, 120) of volatile organics in product water (-13L) from in situ coal gasification (LERC, ERDA).

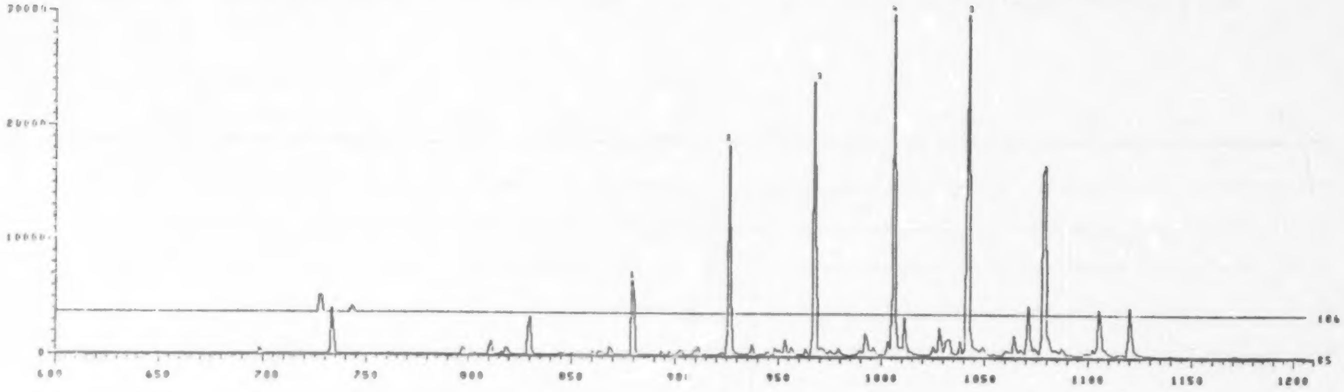


Figure 9. Mass fragmentograms (m/e 186, 85) for volatile organics in product water (-13L) from in situ coal gasification (LERC, ERDA).

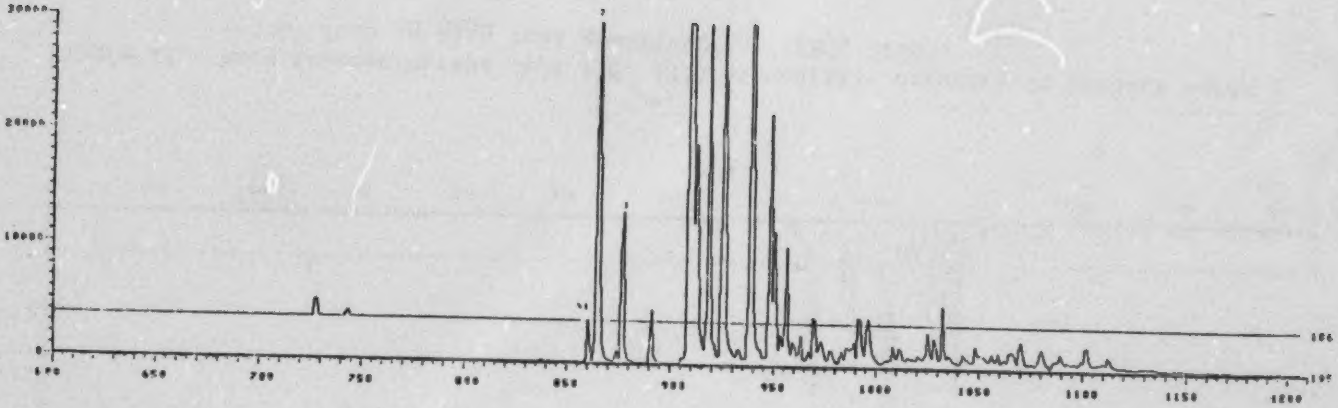


Figure 10. Mass fragmentograms (m/e 186, 105) of volatile organics in product water (-13L) from in situ coal gasification (LERC, ERDA).

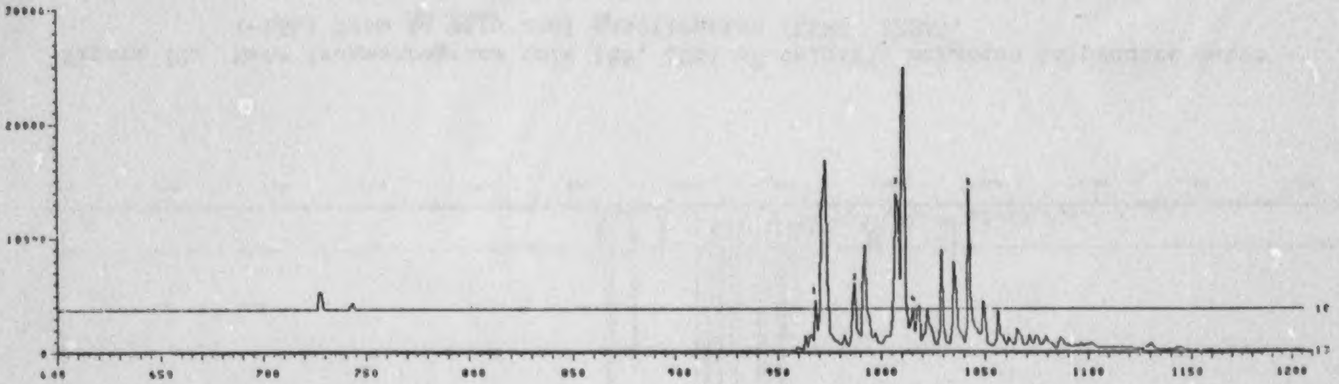


Figure 11. Mass fragmentograms (m/e 186, 131) of volatile organics in product water (-13L) from in situ coal gasification (LERC, ERDA).

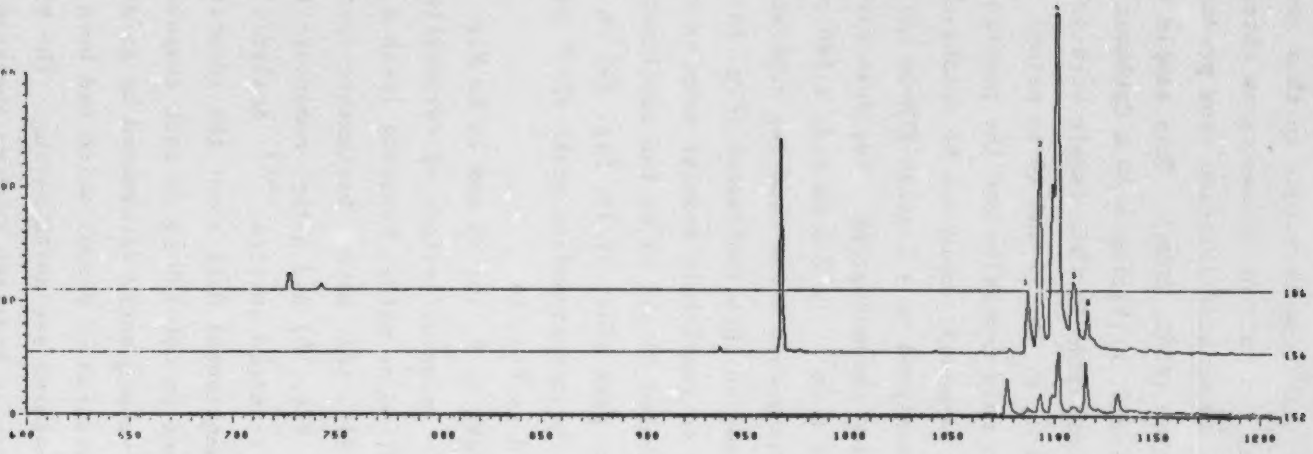


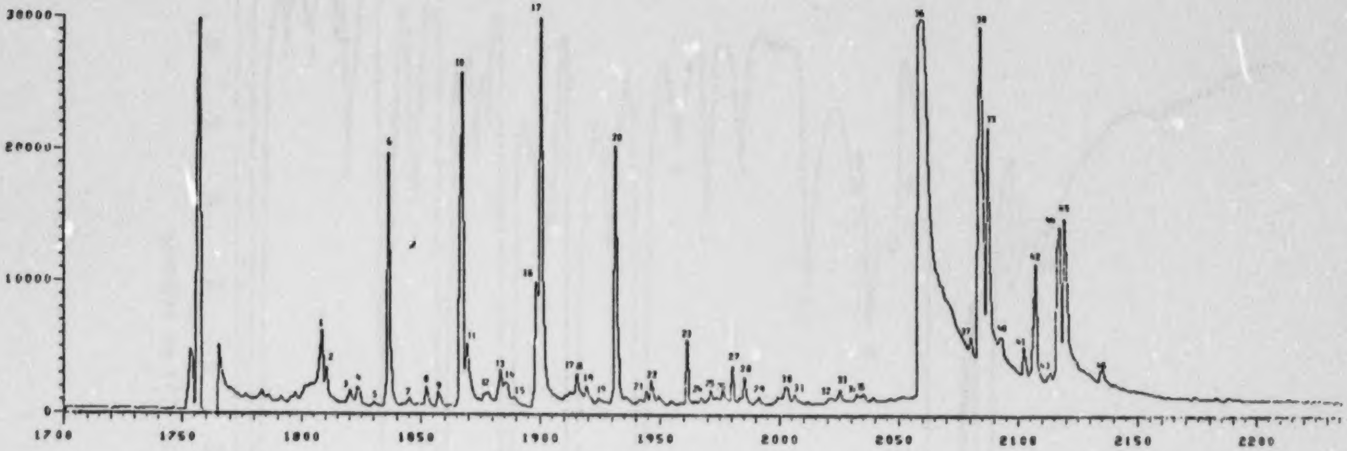
Figure 12. Mass fragmentograms (m/e 186, 156, 152) of volatile organics in product water (-13L) from in situ coal gasification (LERC, ERDA).

using Freon-TF® and methylated using diazomethane. Two samples of product water from an in situ coal gasification process will be discussed here to exemplify the use of the gc/ftir/comp technique in this research program. Figure 13 presents the total ion current chromatogram obtained by gc/ms of the semi-volatile compounds in an acid fraction from product water (-8L) from in situ coal gasification (LERC, ERDA). This sample was analyzed by gc/ms as described in Section 6, utilizing a 60 m Carbowax 20M glass capillary column. Most of the compounds in this sample were identified, although the identification of peaks 1, 6, 10, 17 and 20 as methyl esters of aliphatic carboxylic acids was only tentative and the positions of aromatic substituents on some other compounds could not be established.

This sample was also analyzed on a Digilab FTS-20 gc/ir equipped with a Hewlett-Packard 5700 series chromatograph. The scan rates were 0.5 sec/spectrum at a resolution of 8 cm^{-1} A 2.5 mm i.d. x 180 cm column packed with 10% Carbowax 20M on Chromosorb W was used for separating the mixture. The FID chromatogram obtained on this instrument (Fig. 14) illustrates the need for capillary columns to completely resolve samples of this nature. For instance, the peaks labeled 38 and 39 on the capillary chromatogram (Fig. 13) are a homogeneous peak (Nos. 22/23, Fig. 14) in the packed column FID chromatogram. The corresponding peaks 42-46 in the capillary chromatogram are unresolved in Fig. 14.

The IR spectra for peaks 6, 8, 10, 12 and 14 in Fig. 14 confirm the identity of these compounds as methyl esters of carboxylic acids. The compounds have been identified as methyl benzoate (peak 6, Fig. 15), methyl hexanoate (peak 8, Fig. 18), methyl heptanoate (peak 10, Fig. 17), methyl octanoate (peak 12, Fig. 18) and methyl nonanoate (peak 14, Fig. 19) and compare well with the standard spectra.(41) Analysis of the mixture by gc/ms could not provide unequivocal data about the identity of these compounds. The IR spectra were obtained on ~60-180 ng of each component in the sample. Their concentrations were subsequently determined by gc/ms/comp.

Figure 20 is an IR spectrum of phenol which had been previously identified by gc/ms. Several features are worth noting. The broad peak from 3000-3500 cm^{-1} due to molecular hydrogen bonding observed in condensed phase spectra(43) is absent in this gas phase spectrum. The two peaks



Mass Spectrum No.

Figure 13. Total ion current chromatogram obtained by GC-MS of semi-volatile organics in acid fraction of product water (-8L) in situ coal gasification (LERC, ERDA).

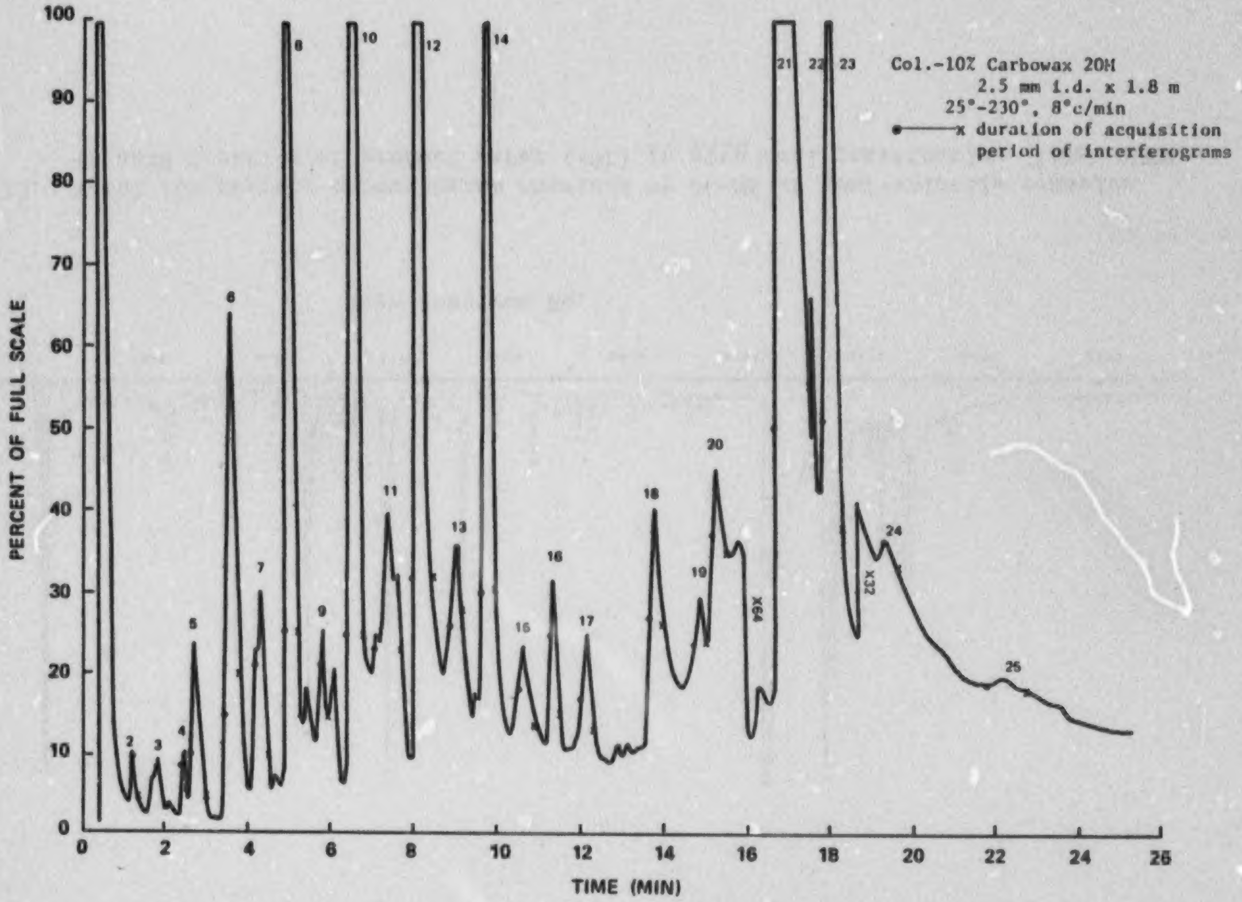


Figure 14. Gas-liquid chromatogram (flame detection) of acid fraction from product water (-8L) obtained during in situ coal gasification.

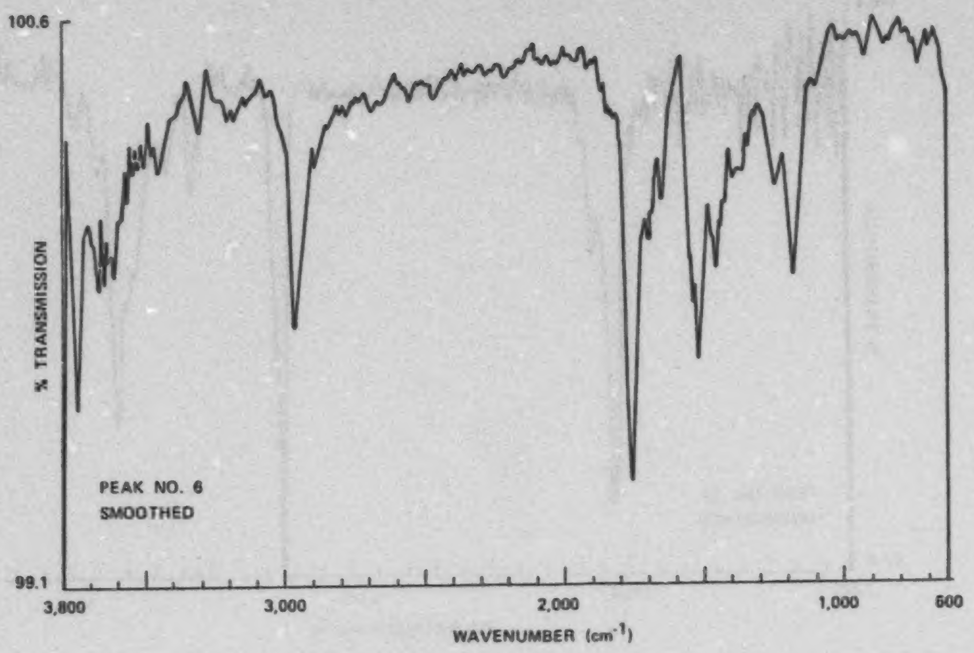


Figure 15. On-the-fly FT-IR spectrum of peak No. 6 (ca. 60 ng) in Fig. 14.

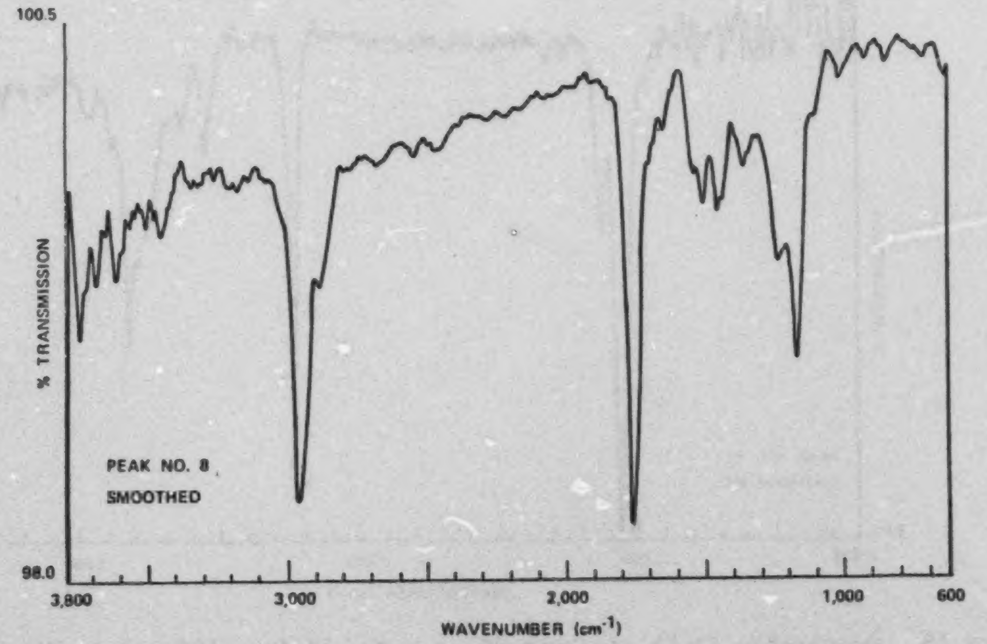


Figure 16. On-the-fly FT-IR spectrum of peak No. 8 (ca. 125 ng) in Fig. 14.

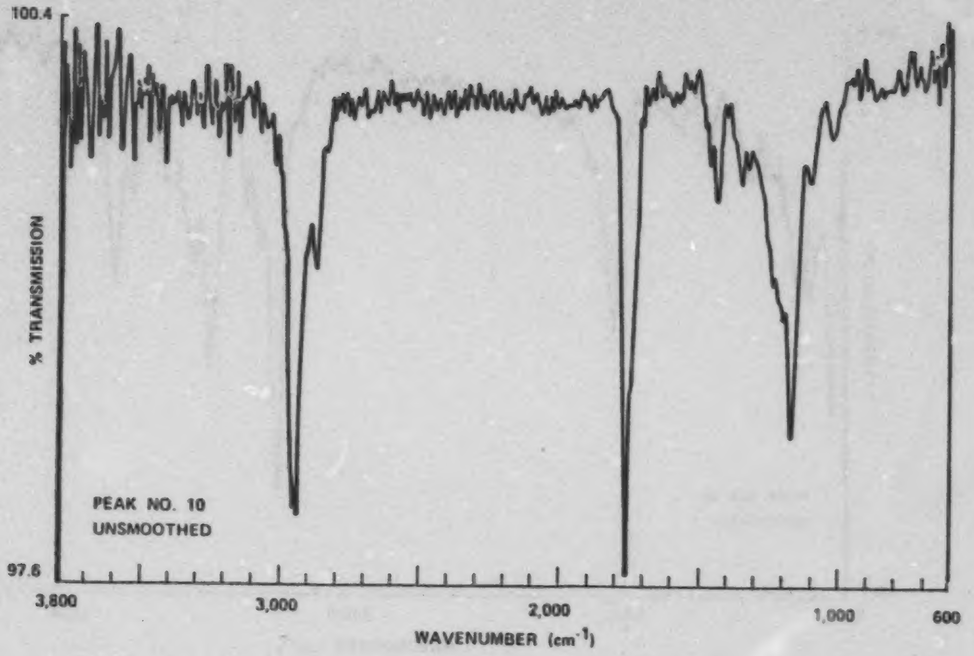


Figure 17. On-the-fly FT-IR spectrum of peak No. 10 (ca. 175 ng) in Fig. 14.

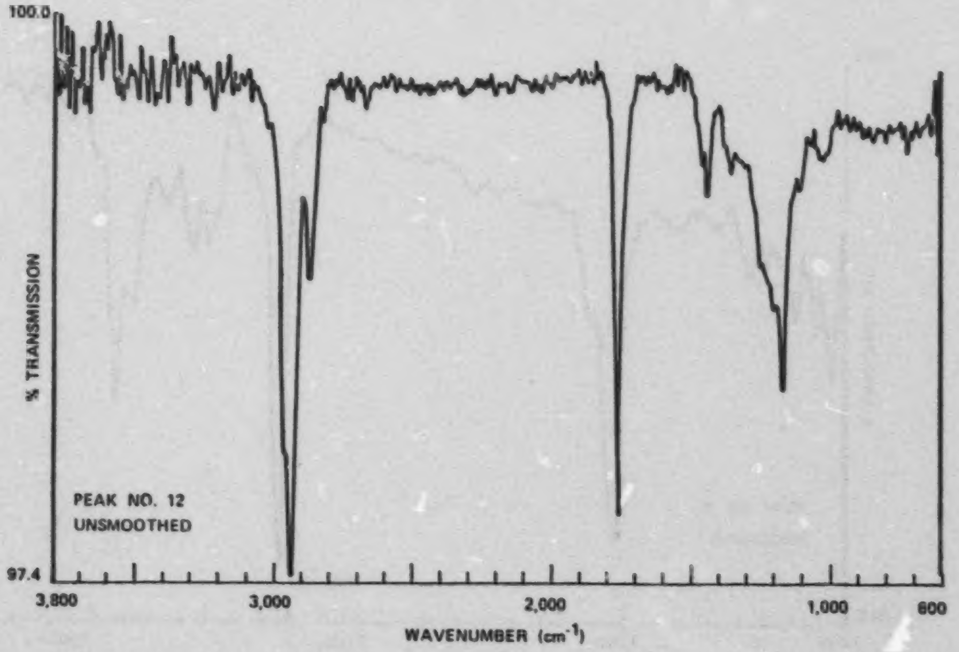


Figure 18. On-the-fly FT-IR spectrum of peak No. 12 (ca. 180 ng) in Fig. 14.

observed between 1175-1300 cm^{-1} are the symmetric and asymmetric CO stretching bands. In condensed phase spectra, this is a broad single band.

Peak 22 had been identified by gc/ms as a dimethylphenol isomer. The gc/ftir spectrum (Fig. 21) confirmed this as a phenol. From the pattern of the overtone in combination bands between 1652-2000 cm^{-1}, it may tentatively be identified as 3,5-dimethylphenol. The standard spectrum for 3,5-dimethylphenol(43) differs from this spectrum at several points, notably the presence of a strong absorbance band at 1310 cm^{-1} and several bands between 1600-1000 cm^{-1} which do not appear in the unknown spectrum. This standard spectrum, however, matched that of the unknown more closely than the spectrum of the other dimethylphenol isomers. Since the standard spectra were run in liquid phase, positive identification could not be made without a gas phase standard spectrum.

Peak 23 (Figure 14) is a cresol isomer according to the gc/ms results. However, the overlap from peak 22 obscured the IR spectrum (Figure 22). With spectral subtraction, this compound could probably be resolved and identified.

Figure 23 illustrates the power of spectral subtraction and smoothing for an extremely weak spectrum. This compound was tentatively identified by gc/ms as methyl-m-toluate and the strong absorbance at 1280 cm^{-1} supports this assignment. The absorbances at 1440, 1290, 1200, 1100 and 750 cm^{-1} match those of the standard spectrum for methyl-m-toluate.(44) The amount of this compound was eventually estimated to be ~30 ng/μℓ injected into the gc/ms.

Table 9 summarizes the semi-volatile organic acids which were identified and confirmed by gc/ftir/comp techniques. The general procedures described above were utilized for confirming the presence of some of the organic constituents present in liquid effluents from energy-related processes.

Another example of a sample analyzed by gc/ms and gc/ftir using a Nicolet 7199 instrument is presented here. The sample was chromatographed using a Varian 3700 gas chromatograph equipped with 180 cm x 0.2 cm i.d. stainless steel column packed with 10% Carbowax 20M with a helium flow rate of 30 cm^3/min. The temperature was programmed from 70-230° at 8°/min. The infrared spectra were collected at 8 cm^{-1} resolution at a rate of 2 scans/sec with every 3 co-added. The light pipe used was a 28 cm x 0.2 cm i.d. (0.8 cm^3/volume) solid gold prototype.

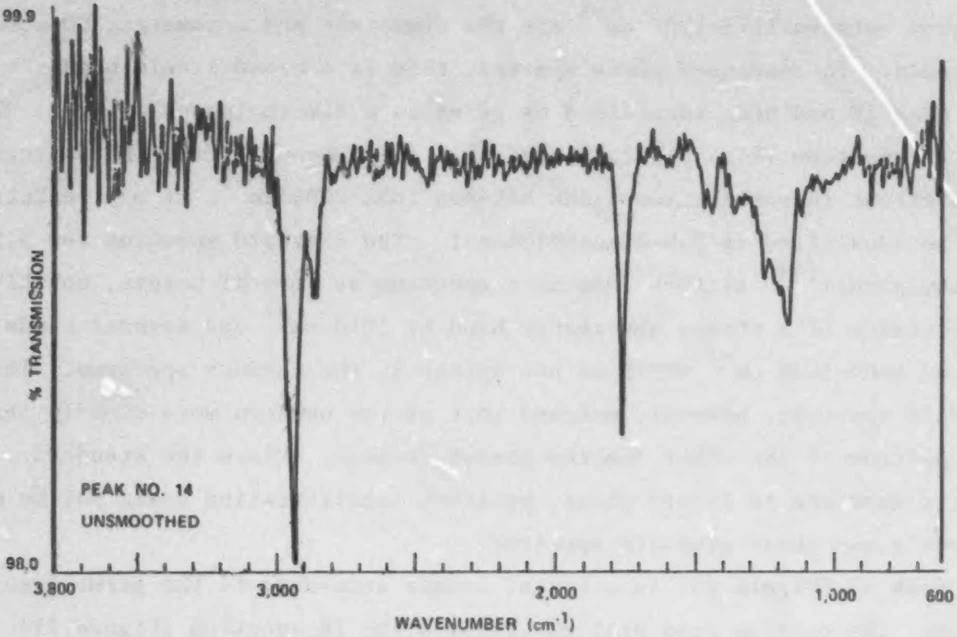


Figure 19. On-the-fly FT-IR spectrum of peak No. 14 (ca. 110 ng) in Fig. 14.

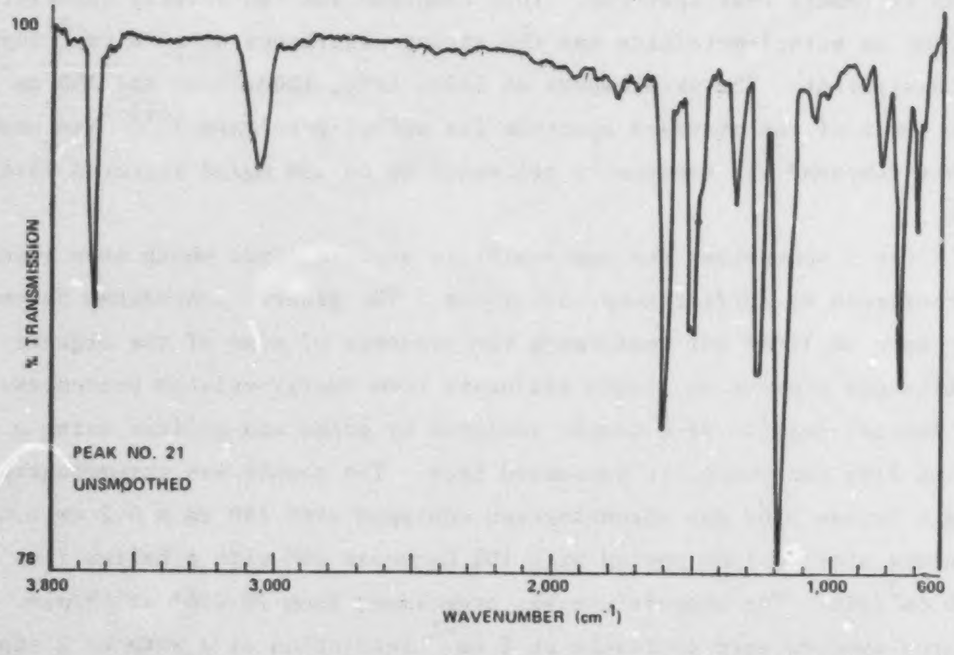


Figure 20. On-the-fly FT-IR spectrum of peak No. 21 (>3 μg) in Fig. 14.

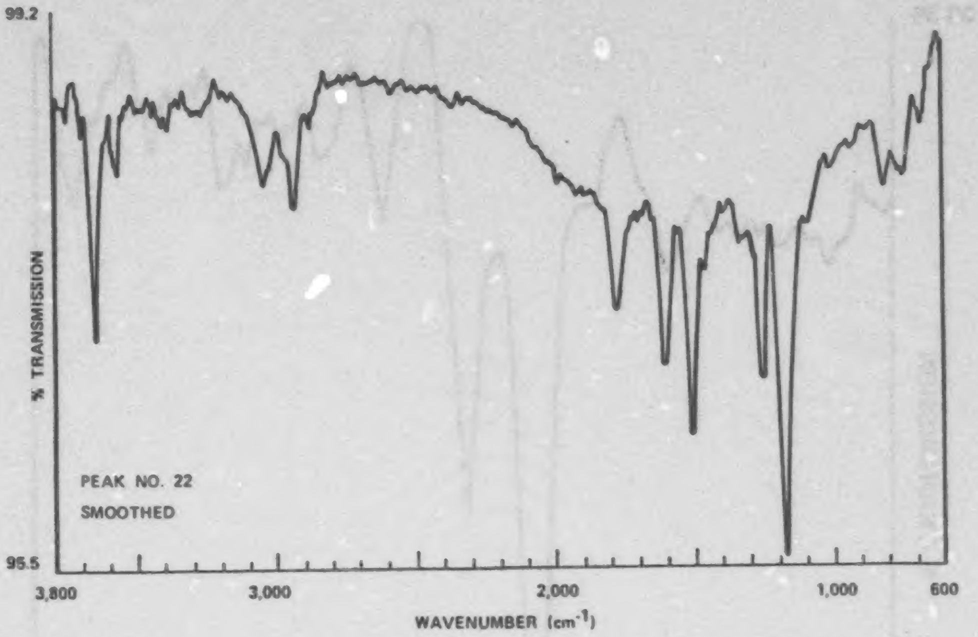


Figure 21. On-the-fly FT-IR spectrum of peak No. 22 (ca. 80 ng) in Fig. 14.

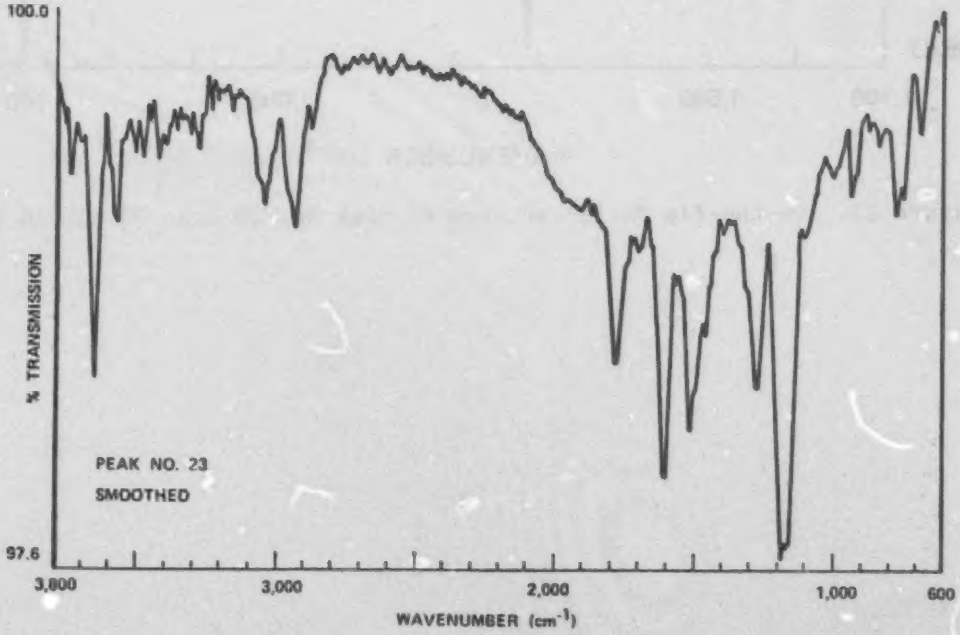


Figure 22. On-the-fly FT-IR spectrum of peak no. 23 (ca. 75 ng) in Fig. 14.

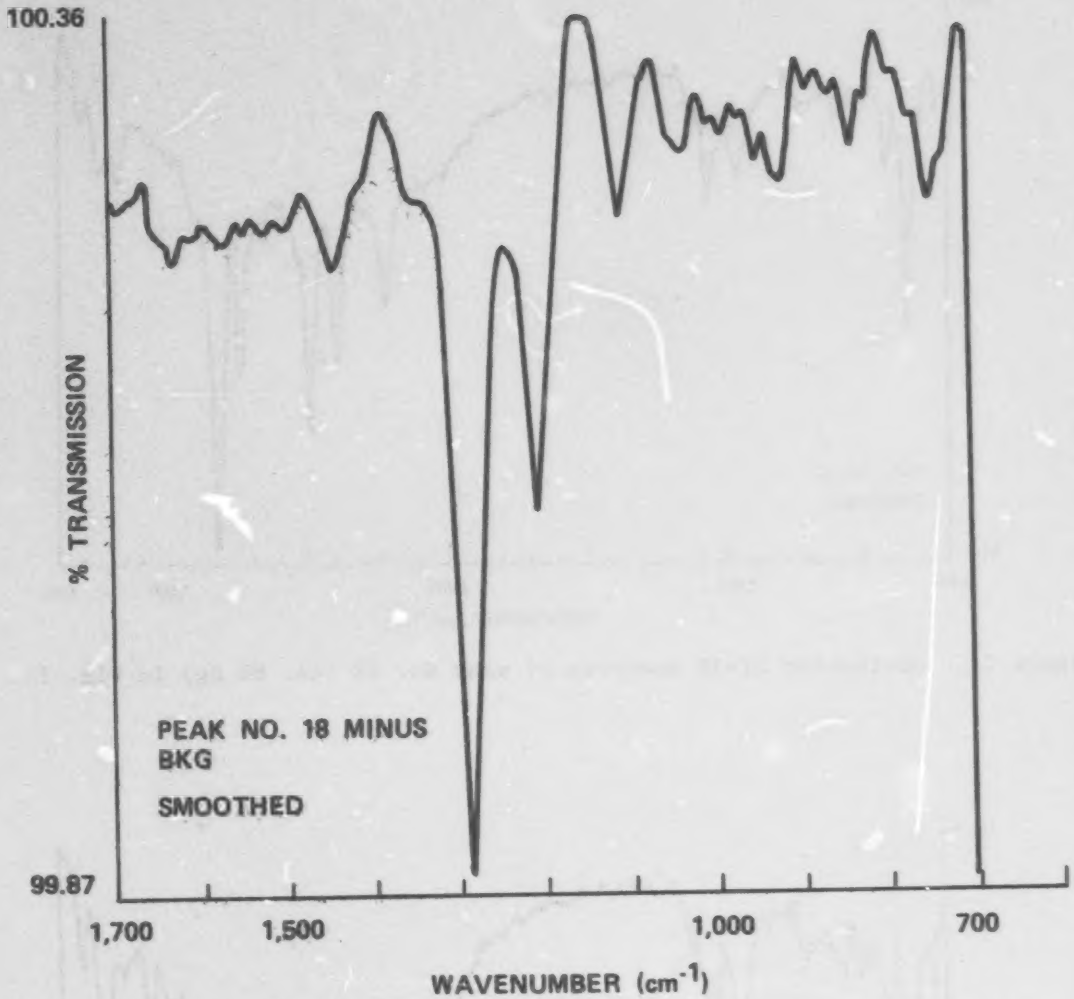


Figure 23. On-the-fly FT-IR spectrum of peak No. 18 (ca. 30 ng) in Fig. 14.

Table 9. SEMI-VOLATILE ORGANIC ACIDS IN PRODUCT WATER (-8L) FROM IN SITU COAL GASIFICATION (LERC, ERDA)[a]

Chromato-graphic Peak No.	Compound	Chromato-graphic Peak No.	Compound
1	methyl butyrate (tent.)	26	5-methyl-3-hexanol
1A	methyl pentanoate	27	2,2-dimethyl-3-pentanol
2	ethyl butyrate	28	heptanol isomer
3	$C_5H_{10}O_2$ (isomer)	31	methyl-m-toluate
3A	methyl-α-methyl butyrate	33	dimethyl methyl benzoate isomer
4	$C_7H_{14}O_2$ (isomer)	34	dimethyl methyl benzoate isomer
5	2-methyl-1,3-dioxane (tent.)	35	dimethyl methyl benzoate isomer
6	methyl hexanoate	36	phenol
8	$C_7H_{12}O$ (isomer)	37	dimethyl phenol isomer
9	2-methyl-2-propyl-1,3-dioxalane	38	dimethyl phenol isomer
10	methyl heptanoate	39	o-cresol
14	anisole	40	isopropyl phenol isomer
17	methyl octanoate	41	C_3-alkyl phenol isomer
17A	$C_8H_{12}O$ isomer	41A	ethyl phenol and cresol isomer
18	$C_8H_{12}O$ isomer and $C_9H_{16}O$ isomer	41B	C_3-alkyl phenol isomer
20	methyl nonanoate	42	xylenol
21	trans-decalin	43	cresol and C_3-alkyl phenol
22	cis-decalin	44	dimethyl phenol
23	methyl decanoate	45	ethyl phenol isomer

(continued)

Table 9 (cont'd)

Chromatographic Peak No.	Compound	Chromatographic Peak No.	Compound
24	phenyl acetate	45A	ethyl phenol isomer
25	methyl benzoate	46	dimethyl phenol isomer

---

[a] Sample extract treated with diazomethane.

Figure 24 is the "chemigram" obtained in real time for this run. The lower trace is the integrated absorbance from 700-3600 cm^{-1} within an absorbance range from -0.002- +0.014. The upper trace is the carbonyl region only (1700-1750 cm^{-1}) to selectively detect the carbonyl-containing compounds expected in the sample. The selectivity is illustrated with the solvent (Freon-TF®) peak at 100 sec which absorbs strongly in the lower trace but presented only a small response in the upper trace. Conversely, the carbonyl containing compounds gave strong peaks at 195, 240, 300 and 335 sec in the upper chemigram. Figures 25-28 are spectra obtained from this analysis. The file number on each spectrum corresponds to the appropriate number along the X axis. In cases where more than one number is listed (e.g., Files 31-35), the spectrum files were co-added. The strong absorbance at 2350 cm^{-1} in each spectrum is an interference due to the unpurged system. Figures 25-28 have been identified as methyl hexanoate, methyl heptanoate, methyl octanoate and methyl nonanoate, respectively. Figure 29 was identified as phenol.

Elemental Composition of Liquid and Solid Effluents

Appendix B presents the elemental constituents in liquid and solid effluents which were detected and quantified by spark-source mass spectrometry and flameless atomic absorption spectrophotometry. The results for the samples listed in Table 3 of Section 5 are provided in Tables B1-B48 (Appendix B).

Organic Composition of Liquid and Solid Effluents

Appendices C and D present the identity and quantity of volatile and semi-volatile organic substances in liquid and solid effluents from *in situ* oil-shale processing, *in situ* coal gasification, and low btu coal gasification.

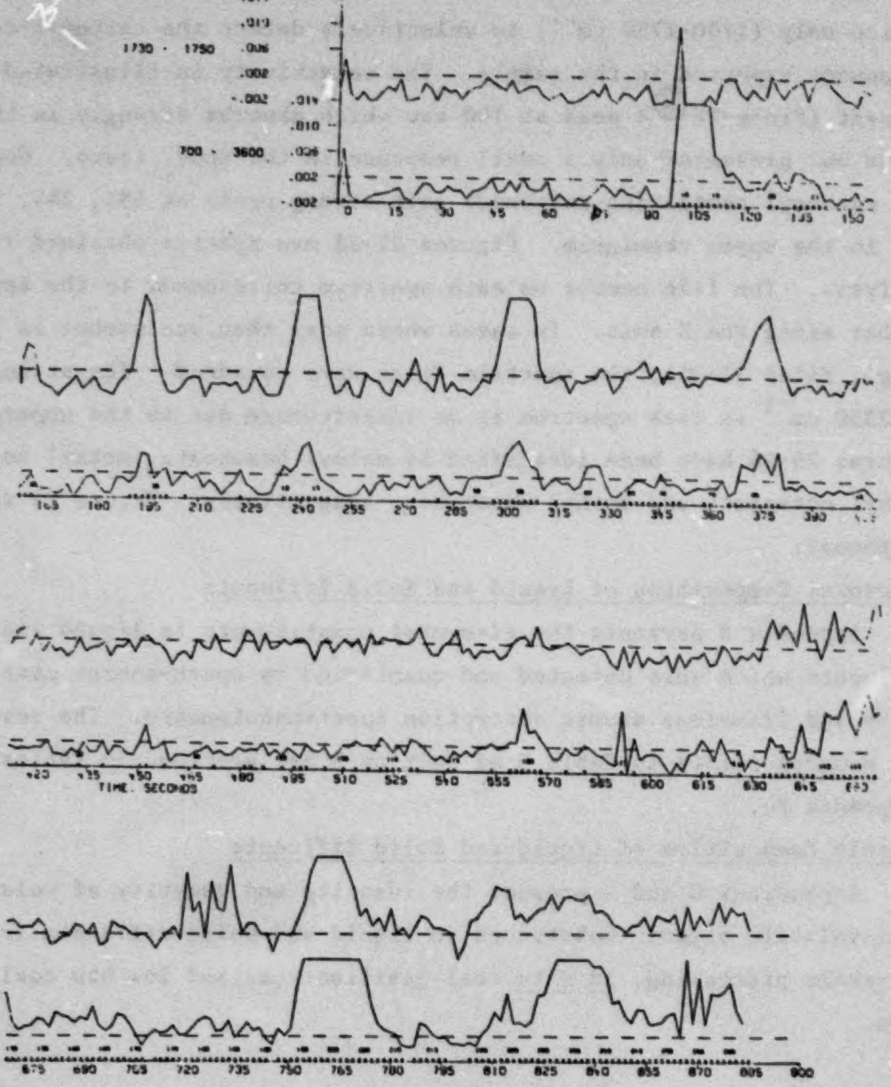


Figure 24. "Chemigram" (ir detection) of acid fraction from product water obtained during in situ coal gasification.

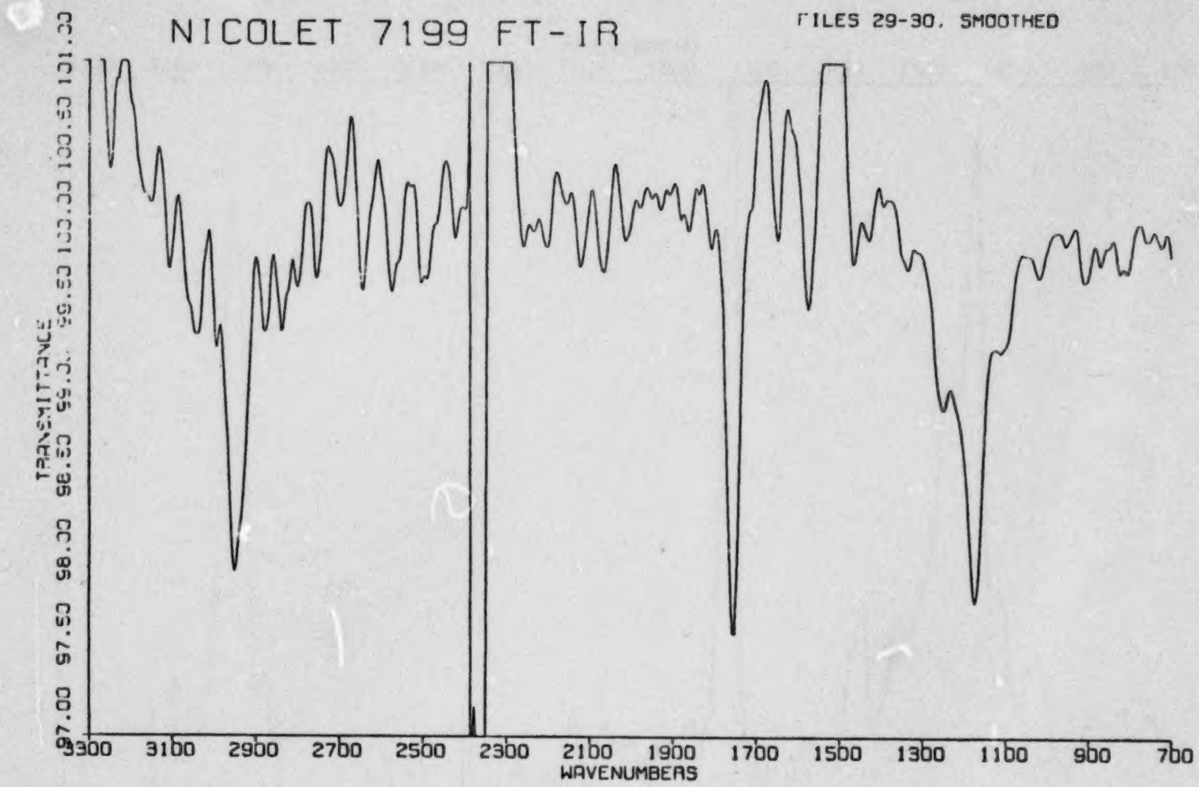


Figure 25. On-the-fly FT-IR spectrum of methyl hexanoate (Files 20-30 of chemigram co-added and smoothed)

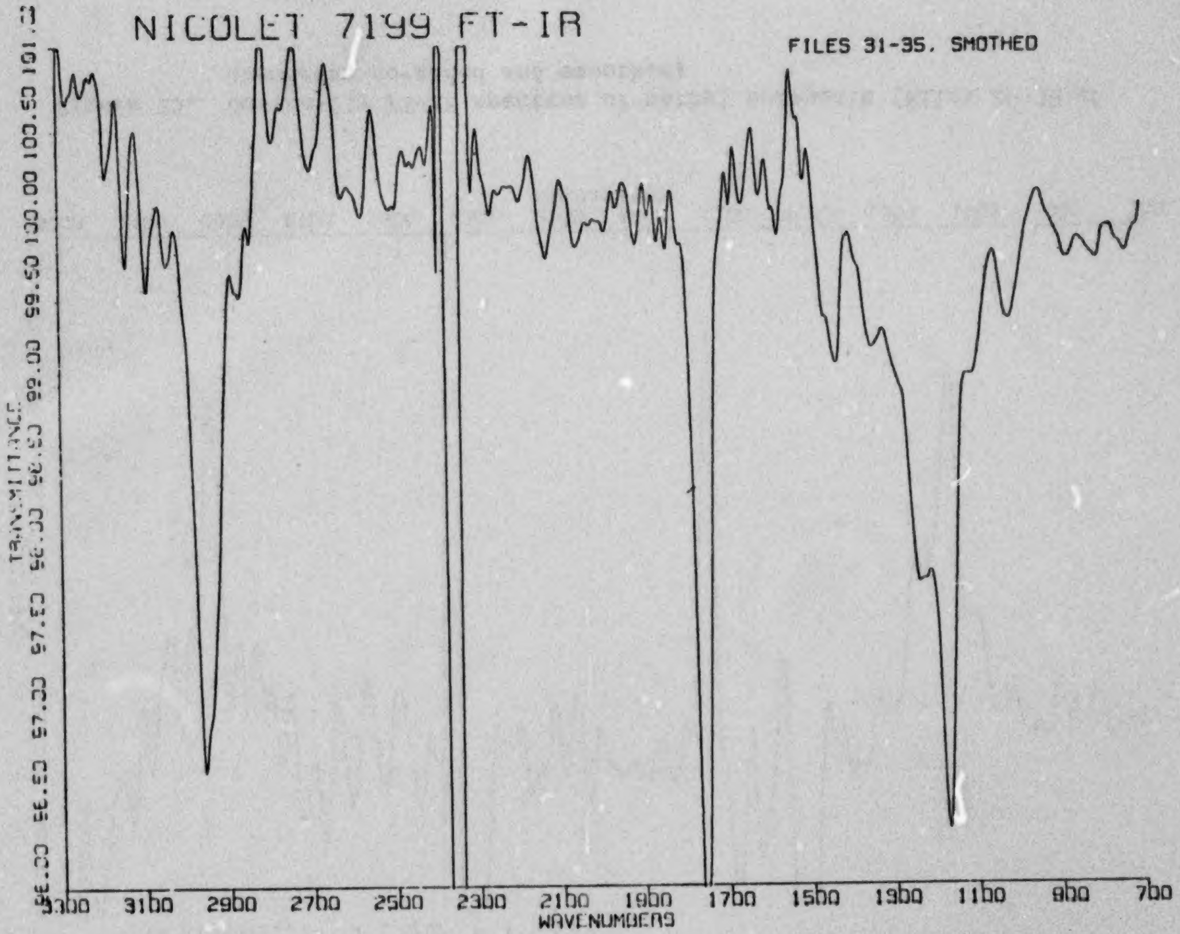


Figure 26. On-the-fly FT-IR spectrum of methyl heptanoate (Files 31-35 of chemigram co-added and smoothed).

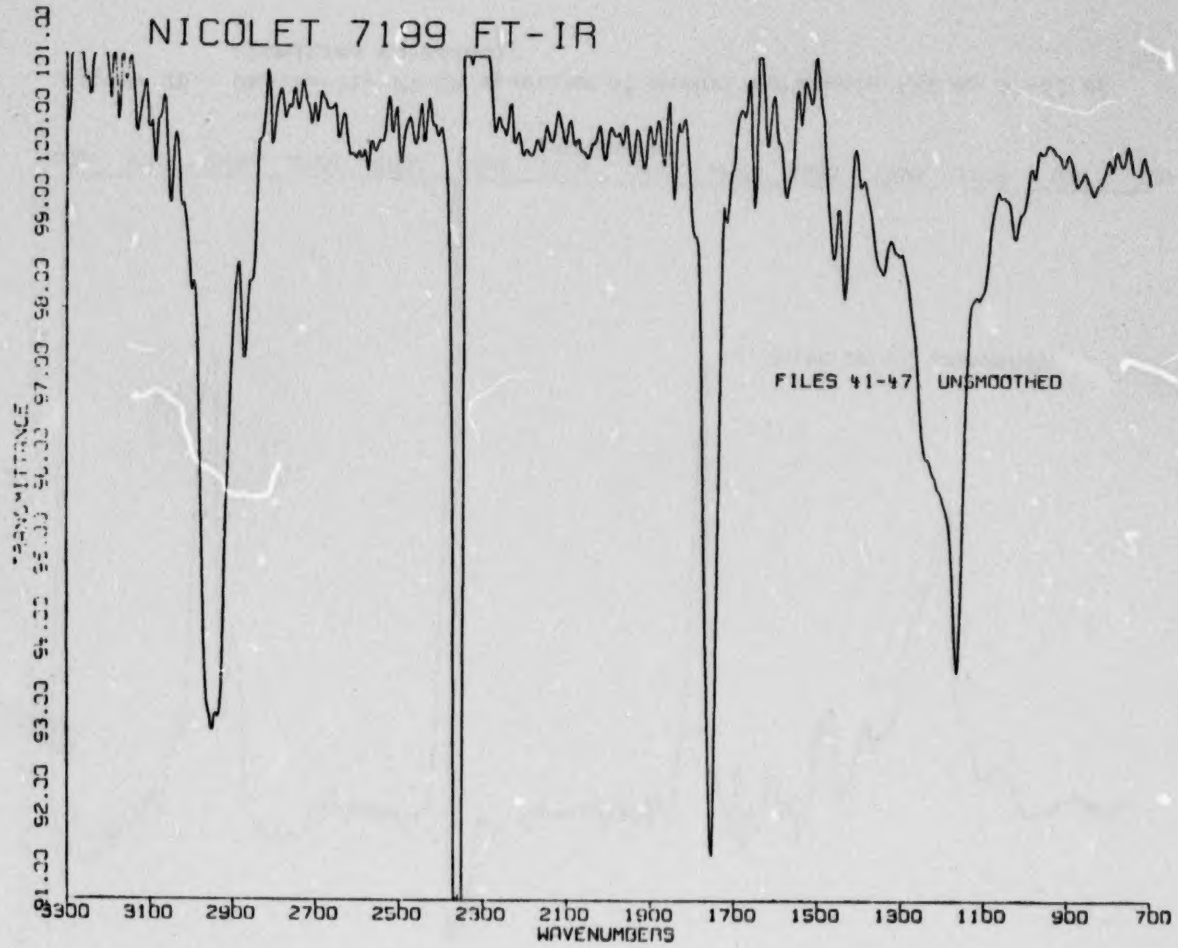


Figure 27. On-the-fly FT-IR spectrum of methyl octanoate (Files 41-47 of chemigram co-added).

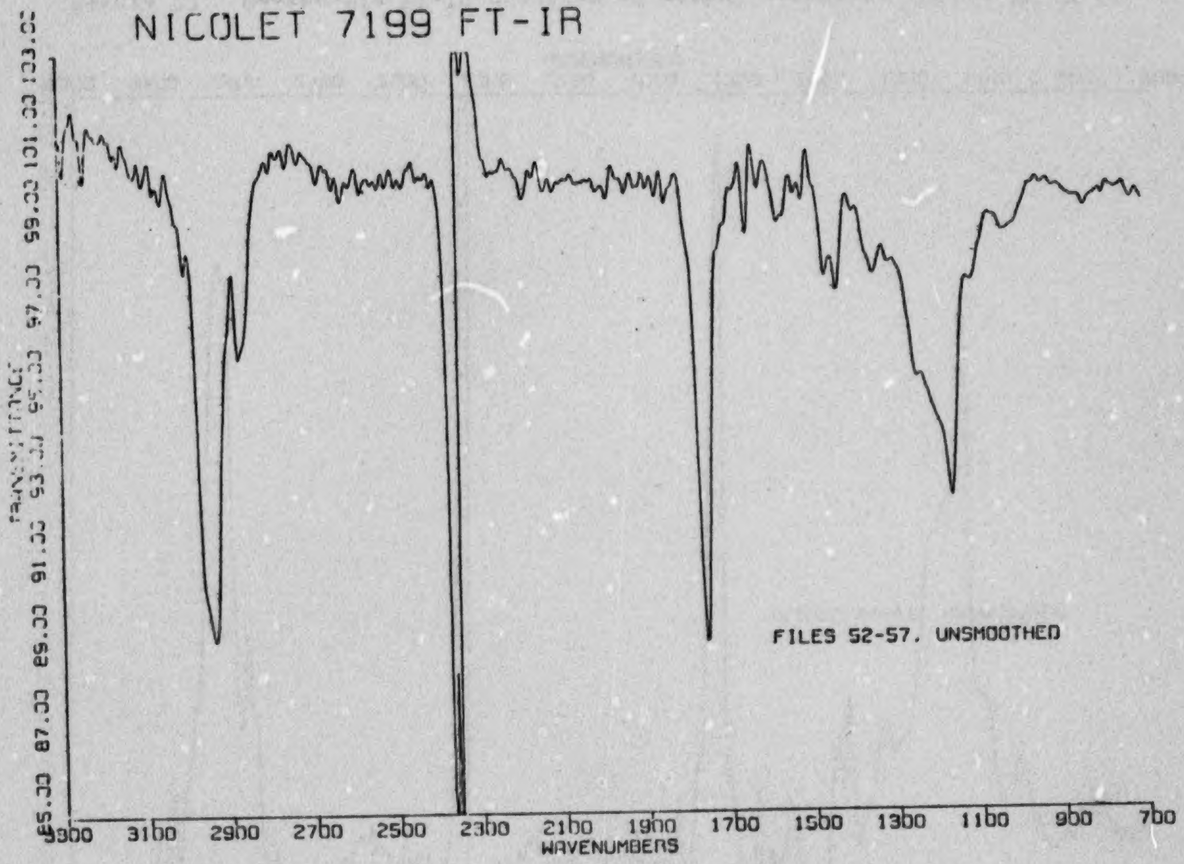


Figure 28. On-the-fly FT-IR spectrum of methyl nonanoate (Files 52-57 of chemigram co-added).

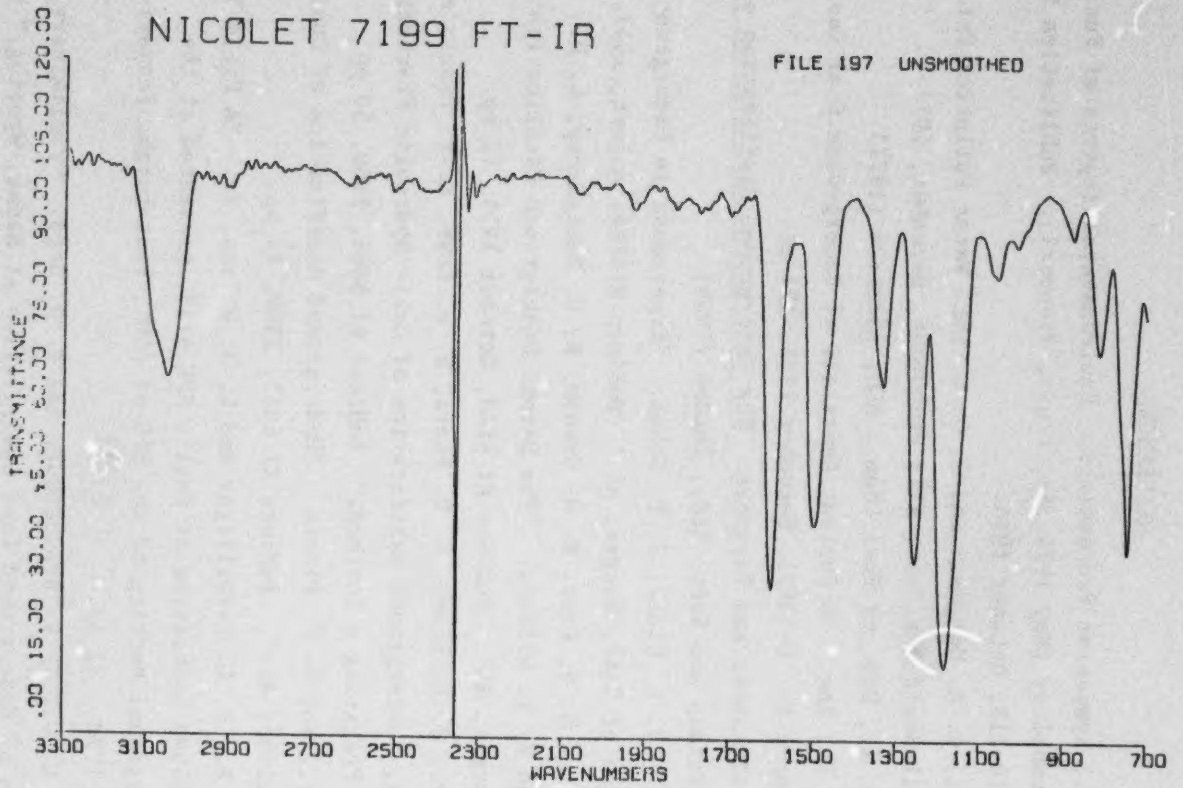


Figure 29. On-the-fly FT-IR spectrum of phenol (File 197 of chemigram).

REFERENCES

1. Ayer, F. A., Symposium Proceedings: Environmental Aspects of Fuel Conversion Technology (May 1974, St. Louis, Missouri). Publication No. EPA-650/2-74-118, October 1974.
2. Ward, J. C., G. A. Margheim and G. O. C. LöF. Water Pollution Potential of Spent Oil Shale Residues, NTIS PB-206808, December, 1971.
3. Hubbard, A. B., Div. of Fuel Chem., ACS, 15:21-24 (1971).
4. Little, A. D., Inc. "A Current Appraisal of Underground Coal Gasification". Report No. C-73671, December 1971, 121 pp.
5. Gibb, Sir Alexander and Partners. The Underground Gasification of Coal, Sir Issac Pitman and Sons, Ltd., London (1964).
6. Dowd, J. J., J. L. Elder, J. P. Cohen. "Experiment in Underground Gasification of Coal, Gorgas, AL." BuMines RI4164, August, 1947, 62 pp.
7. Elder, J. L., M. H. Fies, H. G. Graham, R. C. Montgomery, L. D. Schmidt and E. T. Wilkins. "The Second Underground Gasification Experiment at Gorgas, AL". BuMines RI 4808, October 1951, 72 pp.
8. Capp, J. P., J. L. Elder, C. D. Pears, R. W. Lowe, K. D. Plants and M. H. Fies, "Underground Gasification of Coal--Hydraulic Fracturing as Method of Preparing a Coalbed." BuMines RI 5666, 1960, 50 pp.
9. Capp, J. P., and K. D. Plants. "Underground Gasification of Coal with Oxygen-Enriched Air". BuMines RI 6042, 1962, 14 pp.
10. Raimondi, P., P. L. Terwilliger and L. A. Wilson, Jr. "A Field Test of Underground Combustion of Coal", SPE 4713, presented at the Eastern Regional Meeting of the SPE of AIME, Pittsburgh, Pennsylvania, Nov. 7-9, 1973. 11 pp.
11. Campbell, G. G., C. F. Brandenburg and R. M. Boyd. "Preliminary Evaluation of Underground Coal Gasification at Hanna, Wyoming," BuMines TPR 82, Oct. 1974, 14 pp.

12. Schrider, L. A., J. W. Jennings, C. F. Brandenburg and D. D. Fischer. "An Underground Coal Gasification Experiment, Hanna, Wyoming", SPE 4993, presented at the SPE Fall Meeting of AIME, Houston, TX, Oct. 6-9, 1974, 25 pp.

13. Brandenburg, C. F., D. D. Fischer, G. G. Campbell, R. M. Boyd and J. K. Eastlack. "The Underground Gasification of Subbituminous Coal", presented at the Div. of Fuel Chem., Am. Chem. Soc. National Spring Meeting, Philadelphia, PA, April, 1975, 11 pp.

14. Stephens, D. R., F. O. Beane and R. W. Hill. "LLL In-Situ Coal Gasification Program", Preprint UCRL-78308, Aug., 1976.

15. Campbell, J. H. and H. Washington. "Preliminary Laboratory and Modeling Studies on the Environmental Impact of "In-Situ" Coal Gasification", Preprint UCRL-78303, July, 1976.

16. Meade, W. "The Control of Gas and Liquid Effluents During Hoe Cree Experiment #1", UCID-16984, December, 1975.

17. Schrider, L. A. and J. W. Jennings. "An Underground Coal Gasification Experiment, Hanna, Wyoming", Soc. Pet. Eng. of AIME, No. SPE-4993, 1974, 14 pp.

18. Brandenburg, C. F., R. P. Reed, R. M. Boyd, D. A. Northrop and J. W. Jennings. "Interpretation of Chemical and Physical Measurements from an In-Situ Coal Gasification Experiment", Soc. Pet. Eng. of AIME, No. 5654, 1975, 12 pp.

19. Kubasik, N. P., H. E. Sine and M. T. Volosin, Clin. Chem., 18, 1326 (1972).

20. Kessler, T., A. G. Sharkey, Jr., and R. A. Friedel, Spark Source Spectrometer Investigation of Coal Particles and Coal Ash, Bureau of Mines, Technical Progress Report 42 (1971).

21. Ruch, R. R., H. J. Gluskoter and N. F. Shimp, Occurrence and Distribution of Potentially Volatile Trace Elements in Coal: A Final Report: Illinois Geological Survey Environmental Geology Note 72 (1974).

22. Harstein, A. M., R. W. Freedman and D. W. Platter, Anal. Chem., 45, 611 (1973).

23. "AEI Technical Sheet, Stainless Steel Moulding Die", AEI Tech. Information Sheet, A-2014.

24. Mcrea, J. M., Applied Spectroscopy, 25, 246 (1971).

25. Paulsen, P. J., Robert Alvarex and Daniel E. Kelleher, Spectrochemical Acta, 24B, 535 (1969).

26. Owens, E. B. and N. A. Giardino, Anal. Chem., 35, 1172 (1973).

27. "Quantitative Determination of Impurities by Means of Spark Source Mass Spectrometer", N. W. H. Addink, Mass Spectrometry, Edited by R. I. Reed, Academic Press, London, 1965.

28. "Mass Spectrometric Methods", Richard E. Honig, Trace Analysis of Semiconductor Materials, p. 169, Pergamon Press, New York, 1964.

29. Nicholls, G. D., A. L. Graham, Elizabeth Williams and Margaret Wood, Anal. Chem., 39, 584 (1967).

30. Bellar, T. A., and J. J. Lichtenberg. "The Determination of Volatile Organic Compounds at the μg/ℓ Level in Water by Gas Chromatograph", EPA Rept. No. 670/4-74-009, November, 1974.

31. Zlatkis, A., H. A. Lichenstein and A. Tishbee, Chromatographia, 6, 67 (1973).

32. Dowty, B., D. Carlisle, J. L. Laseter and J. Storer, Science, 187, 75 (1975).

33. Pellizzari, E. D., EPA Quarterly No. 2, Contract No. 68-03-2368, July, 1976.

34. Pellizzari, E. D., J. E. Bunch, B. H. Carpenter and E. Sawicki, Environ. Sci. Tech., 9, 552 (1975).

35. Pellizzari, E. D., B. H. Carpenter, J. E. Bunch and E. Sawicki, Environ. Sci. Tech., 9, 556 (1975).

36. Pellizzari, E. D. "Development of Method for Carcinogenic Vapor Analysis in Ambient Atmospheres". Publication No. EPA-650/2-74-121, Contract No. 68-02-1228, July, 1974.

37. Pellizzari, E. D. "Development of Analytical Techniques for Measuring Ambient Carcinogenic Vapors". Publication No. EPA-600/2-75-076, Contract No. 68-02-1228, 187 pp., November, 1975.

38. Pellizzari, E. D. "The Measurement of Carcinogenic Vapors in Ambient Atmospheres". Publication No. EPA-600/7-77-055, Contract No. 68-02-1228, 288 pp., June, 1977.

39. Pellizzari, E. D. "Analysis of Organic Air Pollutants by Gas Chromatography and Mass Spectroscopy". Publication No. EPA-600/2-77-100, June, 1977.

40. Fales, H. M., T. M. Jaouni and J. F. Babashale, Anal. Chem., 45, 2302 (1973).

41. Eight Peak Index of Mass Spectra. Vol. I (Tables 1 and 2) and II (Table 3), Mass Spectrometry Data Centre, AWRE, Aldermaston, Reading, RG74PR, UK, 1970.

42. Pellizzari, E. D. "Sampling and Analysis for Selected Toxic Substances", EPA Contract No. 68-01-1978, Quarterly Rpt. No. 12, 1977, 130 pp.

43. Silverstein, R. M., G. C. Bassler and T. C. Morrill, "Spectrometric Identification of Organic Compounds, 3rd Ed., John Wiley & Sons, New York, NY, 1974, 339 pp.

44. Sadtler Research Laboratories, "Catalog of Infrared Spectra", Philadelphia, PA.

APPENDIX A

ABSTRACTS OF TECHNICAL REPORTS AND CURRENT PROJECTS ON CHARACTERIZATION AND ASSESSMENT OF EFFLUENTS FROM ENERGY-RELATED PROCESSES

Page

Section I - Oil-Shale Processing. 95

Part I: Technical Reports 95

Part II: Current Projects 106

Section II - Coal Gasification and Liquefaction 109

Part I: Technical Reports 109

Part II: Current Projects 175

Section III - Coal-Fired Power Plants 188

Part I: Technical Reports 188

Part II: Current Projects 208

Section IV - Coal Related Pollution 212

Part I: Technical Reports 212

Part II: Current Projects 220

Section V - Oil Refineries. 227

Part I: Technical Reports 227

Part II: Current Projects 231

Section VI - Tar Sands. 232

Part I: Technical Reports 232

Part II: Current Projects 233

Title: Environmental Consideration for Oil-Shale Development

Authors: Nick Conkle, Vernon Ellzey and Keshava Murthy

Performing Organization: Battelle Columbus Laboratory, 505 King
Avenue, Columbus, OH 43201

Sponsoring Agency: EPA, Office of Research and Development, NERC-RTP
Control Systems Laboratory, Research Triangle
Park, NC 27711

Report No./Journal: EPA-650/2-74-099

NTIS/GPO No.: PB-241-942 Type of Report: Final, 1/74-5/74

Abstract

In this report a preliminary literature survey of environmental considerations is presented which is associated with the development of the shale oil industry in the United States. Oil-shale deposits, mining and pretreatment processes, in situ and ex situ retorting, refuse disposal and produce treatment and usage are reviewed.

This report provides an overall view of the anticipated oil shale industry and the likely technical and environmental problems to be encountered. It provides an insight into the technology likely to be employed in the mining, oil extraction and on site upgrading processes. However, it does not provide any information with regard to the types of waste products in liquid and solid effluents from these processes, nor does it allude to any particular work which has been done in this area. The report clearly indicates that research and development on component identification are requried to eliminate the inadequacy in the data base necessary to evaluate potential environmental problems.

Title: Identification of γ-Valerolactone in Waste Water from an Oil-
Shale _in situ_ Retort
Author(s): F. R. McDonald
Performing Organization: Laramie Energy Research Center, Laramie, WY
Sponsoring Agency: United States Department of Labor
Report No./Journal: Bureau of Mines Report 7918
NTIS/GPO No.: PB-440-098 Type of Report: Government Publication

Abstract

The compound _γ-valerolactone_ was identified in an acid fraction isolated from waste water which was collected from an _in situ oil-shale retort_. _Infrared_, _nuclear magnetic resonance_ and _mass spectrometry_ was used for the identification of a fraction collected from a _gas chromatograph_. In the Laramie Energy Research Center, the research being conducted is to determine the concentration and identification of the components associated with the _in situ_ oil-shale retorting.

Title: Water Pollution Potential of Spent Oil Shale Residues

Authors: J. C. Ward, G. A. Margheim and G. O. Lof

Performing Organization: Department of Civil Engineering, Colorado
State University, Ft. Collins, CO 80521

Sponsoring Agency: Water Pollution Control Research Series, Water
Quality Office, Environmental Protection Agency,
Washington, DC 20460

Report No./Journal EPA WQO Grant No. 14030EDB

NTIS/GPO No.: Unknown

Type of Report: Final Government
Technical, December,
1971

Abstract

Physical properties including porosity, permeability, particle size distribution and intensity of spent shale from three different retorting operations are discussed in this report. Experiments were conducted on each of the spent shales by perparing slurries and determining leachable dissolved solids. Also percolation experiments were conducted on the TOSCO spent shale and the quantities of leachable dissolved solids were determined. The concentrations of ionic constituents (Al, Ba, Br, Cl, CO_3, Cu, Cr, F, Fe, I, K, Mn, NO_3, Pb, PO_4, Zn) were estimated in the initial leachates from the spend shale. Computer programs were written to predict equilibrium concentrations in the leachate from the percolation column. The purpose of the program was to predict the extent of leaching and erosion of spent shale due to natural rainfall and the determination of the composition and concentration of natural drainage from spent shale. The concentrations of ionic species in the runoff from spent

shale were correlated with runoff rate, precipitation intensity, flow depth, slope and water temperature.

Title: Toxic Effects on the Aquatic Biota from Coal and Oil Shale Development

Author(s): R. V. Thurston, Rodney K. Skogerboe and Rosemarie Russo

Performing Organization: Natural Resource Ecology Laboratory,
Colorado State University, Ft. Collins, CO
and Fisheries Bioassay Laboratory, Montana
State University, Bozeman, Montana

Sponsoring Agency: Environmental Protection Agency, Fresh Water
Research Laboratory, Duluth, MN

Report No./Journal: Quarterly Progress Report No. 2, July-September, 1975

NTIS/GPO No.: Unknown   Type of Report: Quarterly Report

Abstract

This project has a very broad overall objective which is to provide information about the effects of pollutants resulting from coal and oil shale extraction and conversion on the aquatic biota. The general aims include: (a) the establishment of a chemical data base for evaluating the potential effect of coal and oil shale extraction on fresh water resources and ecosystems, (b) the use of biology and chemistry field studies to assess the nature and extent of effects on aquatic ecosystems and (c) to determine acute and chronic toxicity in bioaccumulations of contaminants involved. The research plan will provide chemical analysis of effluents from coal and oil shale mining sites, energy conversion sites, and coal gasification operations. Identification of known and potential toxicants resulting from these mining and conversion processes will be performed by field and laboratory bioasssay methods.

During this quarterly period, some information was provided on the analytical methodology and analysis of liquid and solid effluents from the various processes under consideration. Within this report, a section discusses the charcteristics of elemental pollutants derived from coal combustion anc conversion. The objective of this phase of the program is to identify and characterize species which are released into the environment which are known or suspected to be harmful to aquatic biota. The specific objectives are also delineated. These are: (a) the identification of individual compounds and compound classes which are likely to exhibit toxicity; (b) the determination of physical and chemical properties of individual pollutants and pollutant classes; (c) the estimation of the probable amounts of individual pollutants and pollutant classes likely to be released into the environment in conjunction with the full scale coal conversion and/or combustion operation, and (d) the determination of the nature of transformations of primary pollutants.

Fugitive emissions from each source will be fractionated for bioassay and toxicity studies, and fractions which are shown to be toxic will be studied in detail in order to identify and characterize the toxic entity or entities. The approach to be taken is to identify those species of substances which are already known to be toxic and, in those cases where the existence of toxic materials is not reasonbly established, bioassays will be conducted prior to their characterization. It is apparent that the program does not intend to identify all the constituents in these samples, but primarily devote its energies to those which are deemed hazardous to the aquatic biota.

Effluents to be studied in this program are: (1) aqueous effluents from conventional combustion and conversion processes of coal (gasification and liquefaction); (2) leachates from solid waste disposal (e.g., waste coal, char derived from conversion processes, bottom ash from coal combustion. fly ash collected from coal combustion, and airborne particles); and (4) tars and product oils derived from conversion processes.

This report provides preliminary information on method development for the extraction of organic species associated with the various types of effluents mentioned above. The analytical methods currently being developed are clearly going to be used for the extraction and purification of polycyclic organic species associated with these matrices. There is no indication in this report that the volatile and semi-volatile compounds will be examined. Gas chromatography and mass spectrometry will be used for analysis of organic compounds. Packed columns are contemplated for the separation of polynuclear compounds, while glass capillary columns are proposed for separation of organic species recovered from steam condensates of aqueous effluents. A second approach which is discussed is the determination of organics by liquid chromatography. The analysis will include sequential gas charomatography/mass spectrometry followed by identification via mass spectral library search facilities. The researchers are in the process of developing a direct gc capillary column interface to the mass spectrometer.

The elemental constituents in waste effluents will also be analyzed. The techniques will include spark source mass spectrometry, neutron activation analysis, gamma-ray excited energy dispersive x-ray floresence, DC arc emission spectrometry, atomic absorption spectrometry and differential pulse anodic stripping voltametry. The major technique for this study will be spark source mass spectrometry and DC arc emission spectrometry.

In summary, this ongoing program proposes to study the organic and elemental constituents associated with the solid and liquid effluents from several processes. The study is an extensive in-depth evaluation, characterization and quantitation of the composition of constituents in these various matrices associated with the energy-related processes. Although the techniques are rather sophisticated for analysis, the methodology for recovering the extremely volatile and semi-volatile compounds has not been developed and if effort is expended in this area it would be sometime before it could be applied. The study appears to emphasize the larger molecules associated with these effluents (particularly the polynuclear aromatic compounds).

Title: The Disposal and Environmental Effects of Carbonaceous Solid
Wastes from Commercial Oil-Shale Operations
Author(s): Josef J. Schmidt-Collerus
Performing Organization: University of Denver, Denver Research
Institute, Denver, CO 80210
Sponsoring Agency: National Science Foundation, Division of
Environmental Systems and Resources, Washington,
DC 20550
Report No./Journal: NSF-RA-E-74-004
NTIS/GPO No.: PB-231-793 Type of Report: First Annual Report,
January, 1974

Abstract

This report is divided into four general sections. The first part covers background and problems relating to the various parts of the projected research program and discusses summaries of the physiography, geology, constitution of oil-shale and technology of retorting. The second section deals specifically with the NSF (RAND) research program and its various aspects. The third part discusses the experimental data obtained on the program and some preliminary conclusions. Finally the fourth part presents a summary statement of the objectives of the program which is presently under investigation and some of the projected objectives of the extended research effort.

A considerable effort in this program is devoted to the sampling and sample preparation of spent carbonaceous shale, soil vegetation, water, air as well as the extraction and concentration procedures for each matrix. The author indicates that much of the published literature

on methods and procedures for polynuclear compounds does not translate to the extracts generated in this program. Much of the effort is devoted to the analysis of polynuclear compounds present in spent shale as well as soil, plant and water samples. The techniques most commonly used are those which require rather large amounts of organic materials, *e.g.*, thin-layer chromatography, ultraviolet spectroscopy, infrared spectroscopy and high pressure liquid chromatography. The techniques of gas chromatography/mass spectrometry are discussed; however, the report implies that the particular instrumentation utilized in this program requires rather large quantities of organic compounds for analysis (*e.g.*, micrograms).

It is apparent that techniques for the analysis of volatile and semi-volatile compounds have not been devised, nor yet addressed (from private communications with the Principal Investigator it is his intention to address this area). Many of the techniques which are being utilized are not appplicable to these classes of compounds (*e.g.*, infrared, fluorescence, hplc, thin-layer, etc.). The very nature of the compounds, *i.e.*, their volatility and the low levels encountered, precludes the use of these techniques.

Title: Chemical-Biological Characterization of Coal Conversion Liquids

Authors: B. R. Clark, I. B. Reuben; C. H. Hoe; and M. R. Guerin

Performing Organization: Oak Ridge National Laboratory; Oak Ridge, TN
37820

Sponsoring Agency: U. S. Energy Research and Development Administration
and the Environmental Protection Agency

Report No./Journal: Presentation at the 81st national meeting of the
American Institute of Chemical Engineers:
Kansas City, Missouri

NTIS/GPO No.: None **Type of Report:** Abstract

April, 1976

Abstract

Product liquids and organic concentrates obtained from aqueous effluents were chemically fractionated and analyzed chromatographically. The fractions were subjected to biological testing to determine their toxic and mutagenic potentials. Those fractions found to be active were further analyzed in order to focus on specific compounds which may produce the biological activity. Analytical techniques included Gas Chromtography with sulphur and nitrogen selective detectors. Chemical identifications were made from chromatographic and GC/MS data. Some mutagenicity test results from various fractions of coal product oil are presented.

Title of Project: Sorption of Residual Organic Substances in Retort Waters by Spent Oil Shale Residues

Principal Investigator: J. A. Leenheer

Specialty: Water Resources Division

Performing Agency: U. S. Dept. of Interior, Geological Survey,
Denver, CO 80225

Supporting Agency: U. S. Dept. of Interior, Geological Survey, Water Resources Division

Agency's Number(s): CR-00-181

Project Period: 7/74 - 6/75 Funds: FY75 $40,000

Summary

This research program proposes to examine organic solutes in natural surface and ground water in regions of oil-shale and coal development and in retort waters with respect to elemental composition, compound class and physical chemical properties. One of the major objectives will be to develop an organic water quality analytical program which delineates the background concentrations of dissolved and sediment organic materials for surface and ground water in regions of oil-shale and coal development. The overall objective is to determine the capacity of spent oil-shale residues to adsorb and immobilize residual organic substances in retort waters.

The individual species of organics selected for study which will be associated with the surface and ground water in the regions of oil-shale and coal development were not delineated.

Title of Project: Characterization of Contaminants in Oil Shale Residues and the Potential for their Management to Meet Environmental Quality Standards

Principal Investigator: J. J. Schmidt-Collerus

Specialty: Chemistry

Performing Agency: Denver Research Institute, University Park,
Denver, CO 80210

Supporting Agency: U. S. National Science Foundation, Division of Advanced Energy Research and Technology

Agency's Number(s): AEN75-00175-A01

Project Period: 7/75 - 6/76 Funds: FY76 - $75,000

Summary

This research program is directed towards providing information needed for mangement of residual spend shale to minimize environmental impact. The specific objectives of the program include: (1) a determination of the amount and kind of organic components in carbonaceous spent shale and in the process water from retorting operations; (2) the isolation and identification of compounds that are known or suspected to have blastomogenic activity; (3) an investigation of the changes that compounds may undergo in large storage sites, and an investigation of the impact on the environmental quality. This will involve studies on solubilization an leaching by ground and run-off water, volatilization of potential air pollutants, identification of POM present in airborne carbonaceous particulate matter from oil shale processing operations and the effect of possible auto-oxidation on volatilization of organic compounds from waste and their transfer into air.

Title of Project: *In Situ* Oil Recovery from Tar Sand Deposits/
Petroleum and Natural Gas

principal Investigator: C. S. Land and L. G. Marchant

Speciality: Unknown

Performing Agency: U. S. ERDA Laramie Research Center, Laramie,
Wyoming and Sohio Petroleum Company

Supporting Agency: U. S. ERDA; Division of Oil, Gas and Shale
Technology, Washington, DC

Agency's Number(s): Unknown

Project Period: 7/1/70 - 9/30/80 Funds: FY73, $146,000
FY74, $165,000
FY75, $725,000
FY76, $930,000

Summary

The objective of this research program was to develop *in situ* methods applicable for recovering oil from *tar sand* deposits without excessive environmental costs.

Title: The Documentation, Organization and Prioritization of Synthetic
Fuel Related Pollutants and Effects

Author(s): George E. Weant

Performing Organization: Research Triangle Institute, P. O. Box 12194,
Research Triangle Park, NC

Sponsoring Agency: U. S. Environmental Protection Agency, Industrial
and Environmental Research Laboratory, Research
Triangle Park, NC

Report No/Journal: July, 1975

NTIS/GPO No.: Unknown Type of Report: Technical (Task Order)

Abstract

The objective of this task order was to provide an extensive literature survey in order to identify, classify and prioritize pollutants associated with fuel processes and fuels. The data base which had identified specific pollutants was obtained from literature reports. Each pollutant was evaluated according to the degree of toxicity or biological effect. This report contains a list of pollutants associated with coal, coking, gasification and liquefaction and oil-shale processing. The relative toxicity, physical and chemical data on these pollutants are presented. Classification is by media discharge, i. e., the pollutants are categorized according to their emission via air, water or solid from the energy-related process.

This report lists both elemental compounds and organics. Upon inspection of these data it is apparent that much of the work has been in coal gasification and liquefaction and that a paucity of data is available for oil-shale processing.

Title: Mass Spectrometric Analytical Services and Research Activities
to Support Coal Liquid Characterization Research

Authors: Stewart E. Scheppele

Performing Organization: The Oklahoma State University; Department
of Chemistry; Stillwater, OK 74074

Sponsoring Agency: The United States Energy Research and Development
Administration (Contract No. E(34-1)-0020)

Reprot No./Journal: BERC-0020-4

NTIS/GPO No.: Unknown Type of Report: Quarterly
3/9-6/8/76

Abstract

Medium and low resolution, field ionization and high resolution 70-eV electron impact mass spectral data were obtained for 38 GPC fractions for an HRI coal-derived liquid by memebers of the separation and characterization group at the Bartlettsville Energy Research Center. Empirical formulas were deduced from the high resolution electron impact data. The field ionization data were acquired for eventual calculation of quantitative distributions for the HRI coal-derived liquid.

The field ionization mass spectral data obtained for the GPC fractions from a Synthoil sample are being converted into quantitative compositional data for this coal-derived liquid. In conjunction with the sub-committee ASTM D-2, this author analyzed a blend of aromatic hydrocarbons obtained from 12 crude oils. A paper describing their investigations of field ionization sensitivities entitled "Determination of Field Ionization Sensitivities for the Analysis of Coal Derived Liquids and their Correlation with Low Voltage Electron Impact Sensitivities" has been submitted to Analytical Chemistry.

Title: Characterization of Coal Liquids Derived from the H Coal Process

Authors: S. A. Holmes; P. W. Woodward, G. P. Sterm, Jr.; J. W. Vogah, and J. A. Dooley

Performing Organization: Bureau of Mines; Bartlettsville, OK

Sponsoring Agency: U. S. Energy Research and Development Administration
Bartlettsville Energy Research Center
Bartlettsville, OK

Report No./Journal: EERC/RI76/10

NTIS/GPO No.: Type of Report: Annual; November, 1976

Abstract

Compositional data of coal liquid products derived from the H coal process were obtained. Two products, one from the fuel oil mode of operation and the other from the Syncrude mode of operation were prepared by Hydrocarbon Research Incorporated from Illinois No. 6 coal. The compositional data of these products were tabulated and characteristics of materials were discussed. Separation and characterization methods as developed by the Bureau of Mines API Research Project 60 for characterizing heavy ends of petroleum were used in analyzing coal liquid distillates within the boiling range 200-500°C. Distillates falling below 200°C were separated and analyzed using chromatographic and spectral techniques.

Title: Organic Constitutents in Process Streams of a Solvent Refining Coral Plant

Authors: Michael R. Peterson

Performing Organization: Radiological Sciences Department
Battelle Northwest Laboratories
Richland, WA 99352

Sponsoring Agency: U. S. Energy Research and Development Administration [E(45-1)-1830]

Report No./Journal: ENWL-B470

NTIS/GPO No.: None

Type of Report: Progress;
December, 1975

Abstract

This report describes some initial studies aimed at characterizing the composition of product streams in a solvent refined coal plant. In studies to data they have identifed about 50 of the major organic compounds in various process streams and in the solvent refined fuel product. Polycyclic hydrocarbons, phenols and quinolines were found to be the main classes of organic compounds present. The solvent refining coal plant is a 50 ton per day pilot plant operated under ERDA Contract by the Pittsburg and Midway Coal Mining Company located near Fort Lewis, WA.

The techniques of sample preparation included sample extraction with benzene into neutral, acid and basic fractions. The components in each of these extracts were then characterized using gas chromatography on two different liquid phases, SP-1000 and SP-2100, and dual flame ionization detector. Retention times of peaks found in each fraction were cross-checked against retention times of known compounds. A

suitable match of retention times on each phase was taken as proof of the identity of the unknown peak in the sample. Some of the extracts were analyzed using gas chromtography/mass spectrometry. The results from the flame ionization runs were verified using gc/ms and many minor components were identified using computer searching of mass spectral libraries.

The authors believe that of the coal, tar, and hydrogenation products of coal which have been studies, about 1,000 of the estimated 10,000 compounds have been identified. The major peaks in the gas chromatography of the straight process naphtha were identified as polynulcear aromatics and some simple phenolic compounds.

Title: Functional Composition of Neutral Oxygen Compounds of Primary Coal Tar

Authors: Z. A. Rumyantseva, E. P. Buryakova, Z. M. Perednikova, I. N. Drizina, N. M. Karavaev

Performing Organization: USSR

Sponsoring Agency: USSR

Report No./Journal: Khimiya Tverdogo Topilva No. 3: 94102 (1973)

NTIS/GPO No.: None **Type of Report:** Publication

Abstract

A study was made of the neutral oxygen compounds of tar from semi-coking of soft coal. The bulk of the neutral oxygen compounds are hydroxyl and carbonyl compounds. Monoatomic bicyclic phenols with weakly acidic properties form stable intermolecular hydrogen bonds among themselves and with carbonyl compounds and are present in the tar as polyassociates. The primary techniques employed were alumina column chromatography and infrared spectroscopy.

Title: Influence of Synthane Gas Fire Conditions on Effluent and Product Gas Production

Authors: David V. Nakles, M. J. Massay, A. J. Forney, W. P. Hances

Performing Organization: Pittsburgh Energy Research Center
Energy Research and Development Administration
Pittsburgh, PA

Sponsoring Agency: U. S. Energy Research and Development Administration

Report No./Journal: PERC/RI-75/6

NTIS/GPO No.: Unknown **Type of Report:** Progress Report

December, 1973

Abstract

This report presents the conditions for the operation of a steam oxygen gasification of coal by the Synthane process and others at the Pittsburgh Energy Research Center. The report is particularly useful since it presents the various characteristics of the operation of a steam oxygen gasifier.

Title: Evaluation of Pollution Control in Fossil Fuel Conversion Processes. Liquefaction: Section II. SRC Process

Author: C. E. Jahnig

Performing Organization: Exxon Research and Engineering Co., P. O.
Box 8, Linden, NJ 07036

Sponsoring Agency: EPA, Office of Research and Development, NERC-RTP
Control Systems Laboratory, Research Triangle
Park, NC 27711

Report No./Journal: EPA-650/2-74-009-F

NTIS/GPO No.: PB-241-792 Type of Report: Final (Task) March, 1975

Abstract

This report discusses the analysis of the solvent refined coal (SRC) process of the Pittsburgh and Midway Coal Mining Co. It includes estimates on the quantitites of solid, liquid and gaseous effluents, where possible. The concentration of 43 elements in the SRC product is given and compared to the coal feed. The instrumental techniques used for analyzing the elements were: atomic absorpiton, neutron activation and flame emmission. The report points out the need for the determination of the trace elements in the products during liquefaction and gasification and the need to do complete balances. In the SRC plant, many of the effluents are from conventional operations such as process furnaces, utility boilers, waste water treating and ash disposal.

The examination of organic constitutents in liquid and solid effluents is briefly discussed. The determination of the individual compounds appearing in the waste effluents of this process was not performed.

Title: Analyses of Tars, Chars, Gases and Waters Found in Effluents
from the Synthane Process

Authors: A. J. Forney, W. B. Hanes, S. J. Gasior, G. E. Johnson and
J. P. Strakey, Jr.

Performing Organization: Bureau of Mines, Pittsburgh, PA

Sponsoring Agency: Department of Interior

Report No./Journal: TPR-76 January, 1974

NTIS/GPO No.: Unknown Type of Report: Government Publication

Abstract

This program has conducted extensive studies on the various effluents found in the Synthane coal to gas process. Elemental analysis of water and gas streams was performed using spark source and electron impact mass spectrometry. Accoring to the authors, the results show that additional research is needed on water.

Title: Effect of Additives on the Gasification of Coal in the Synthane
Gasifier

Authors: A. J. Forney, W. P. Hanes, S. J. Gasior, R. F. Kinney

Performing Organization: Pittsburgh Energy Research Center, Pittsburgh, PA

Sponsoring Abency: ERDA, Washington, DC

Report No./Journal: Energy Sources, 2, 1 (1975)

NTIS/GPO No.: Unknown Type of Report: Literature Publication

Abstract

In this program several calcium compounds were added to coal which was gasified in the Synthane laboratory gasifier at Bruceton, PA. Limestone, slate lime and quicklime all increased the reactivity of the coal. The quality of the polluted water that is condensed after the gasification process is apparently also changed by these additives. Future work in this area will include the determination of the constituents in the polluted water.

Title: Mass Spectrometric Analysis of Product Water from Coal Gasification

Authors: C. E. Schmidt, A. G. Sharkey, Jr. and R. A. Friedel

Performing Organization: Pittsburgh Energy Research Center, Pittsburgh, PA.

Sponsoring Agency: The Bureau of Mines, Advancing Energy Utilization Technology Program, U. S. Department of Interior

Report No./Journal: TPR-86

NTIS/GPO No.: Unknown **Type of Report:** Government Technical Progress Report

Abstract

This report presents information on condensate waters from the Bureau of Mines Synthane process for coal gasification. Investigations were conducted using mass spectrometric methods to determine organic contaminants. Waters from the gasification of 6 coals were extracted with methylene chloride yielding 0.6-2.4 wt. percent extractable material. Using high resolution mass spectrometry, combined gas chromatography/mass spectrometry, and low voltage mass spectrometry, 60-80% of the extract was identified as phenolics. Twenty organic contaminants were identified and were present in the condensate waters from each coal gasified. The relative distribution in the condensates was nearly the same for the 6 coals gasified under various conditions. Phenols were the most abundant compounds in all cases.

Because of the methodology employed in the preparation of the water sample for analysis by mass spectrometry or gas chromatography/mass spectrometry, the volatile vapors present in the waters were not included

in these analyses. The extremely volatile compounds which might be present in the aqueous condensates would be lost in the sample work-up during the evaporation or concentration of methylene chloride.

Title: Mass Spectrometric Analysis of Coal-Tar Distillates and Residues

Authors: J. L. Shultz, R. A. Friedel and A. G. Sharkey, Jr.

Performing Organization: Pittsburgh Energy Research Center, Pittsburgh, PA

Sponsoring Agency: U. S. Department of the Interior, Bureau of Mines

Report No./Journal: RI-7,000

NTIS/GPO No.: Unknown

Type of Report: Government Technical Progress Report

Abstract

This paper discusses the high resolution mass spectrometric analyses of naphthalene and anthracene oils, heavy creosote, and 3 fractions of a pitch. The average molecular weight, aromaticity and mean structural unit were determined for each fraction. The investigation of each fraction of coal-tar has resulted in semi-quantitative data for 38 structural types and a carbon number distribution listing for the alkyl derivatives. Molecular weights of 10 of these structural types had indicated ring systems which were not previously reported in products from high temperature carbonization of coal. Two structures are polynuclear aromatic hydrocarbons, two are oxygen containing compounds, one contains sulfur and five are nitrogen containing compounds.

The purpose of the report was to confirm and extend the data obtained by other chemical and spectroscopic techniques.

Title: Analytical Method for Polynuclear Hydrocarbons in Coal Tar
Authors: H. Matsushita, Y. Esumi, A. Suzuki and T. Handa
Performing Organization: Unknown
Sponsoring Agency: Unknown
Report No./Journal: Jap. Anal., 21(11), 1471-1478 (1972)
NTIS/GPO No.: None Type of Report: Literature Publication

Abstract

This report presents a new analytical method for the analysis of polynuclear hydrocarbons in coal tar. The technique involves extraction of the hydrocarbon by liquid-liquid partition, spearation of the hydrocarbons into individual components by two dimenstional dual band thin-layer chromatography and spectrofluorometric analyses of these components. Environmental samples were also examined using gas chromatography combined with a microwave spectrometric detection system.

Title: Mass Spectrometric Analyses of Streams from Coal Gasification and Liquefaction Processes

Authors: A. G. Sharkey, Jr., J. L. Schultz, C. E. Schmidt and R. A. Friedel

Performing Organization: Pittsburgh Energy Research Center, Pittsburgh, PA

Sponsoring Agency: U. S. Energy Research and Development Administration, Pittsburgh, PA

Report No./Journal: PERC/RI-75/5

NTIS/GPO No.: Unknown Type of Report: Government Technical Progress Report, November, 1975

Abstract

Analysis of the streams from the Pittsburgh Energh Research Center's Synthane and Synthoil processes was reported. Streams from coal gasification and coal hydrogenation processes were outlined in this report and examples were given for the analysis of coal, gas, oil and tar process water. Techniques used were mass spectrometry, gas chromatography/mass spectrometry and spark source mass spectrometry. Data were presented on: (1) analysis of trace and minor elements in coals; (2) the major components in gas from gasification of coal; (3) trace components in the gas from coal gasification; (4) the major structural types in heavy oil and tar fractions from the Synthoil process, (5) organic sulfur compounds from coal hydrogenation; (6) sulfur compounds in the products from multi-pass hydrogenation of an Indiana No. 5 coal; (7) the catalytic hydrosulfurization process; (8) the analysis of benzene-

soluble tar; and (9) the trace elements in a condensate from an Illinois No. 6 coal gasification test run.

Title: Relation of Coal Characteristics to Coal Liquefaction Behavior

Authors: P. H. Given, W. Spackman, A. Davis, P. L. Walker and H. L. Level

Performing Organization: Pennsylvania State Unviersity, University Park, PA

Sponsoring Agency: Unknown

Report No./Journal: ERDA Research Abstracts, July, 1975 Abstract 00710

NTIS/GPO No.: None Type of Report: Literature Publication

Abstract

In this study various characteristics of coal (rank, petrographic composition, geological history an composition of the inorganic constituents) were studied systematically to determine their relevance to liquefaction behavior of coals. A continous flow reactor, batch autoclaves, low pressure reaction vessels and other equipment were used in this investigation. The report contains the following topics: (1) Sample Collection and Characterization; (2) Liquefaction Behavior of a Series of Coals from Appalachia; (3) Major, Minor and Trace Elements in Liquid Products and Solid Residues from Catalytic Hydrogenation of Coals; (4) Mechanistic Studies; (5) Studies with Hydrogen Transfer Techniques; (6) Use of Differentiation Scanning Colorimetry for Evaluating Coals for Liquefaction Studies; (7) Characterization of Mineral Matter from Coals by Scanning Electron Microscopy; and (8) Preparation of Maceral Concentrations for Liquefaction Research.

Title: Characterization of Nitrogen Compounds in Tar Produced from Underground Coal Gasification

Authors: S. B. King, C. F. Brandenburg and W. J. Lanum

Performing Organization: Energy Research and Development Administration, Laramie, WY

Sponsoring Agency: U. S. Energy Research and Development Administration

Report No./Journal: Pg. 131-139, ACS 169th National Meeting, Washington, DC, 1975

NTIS/GPO No.: None   **Type of Report:** Abstract

Abstract

The composition of coal tar produced from in situ coal gasification is discussed as part of the monitoring program of the underground migration of these organic fluids. The program proposes to determine what effect they may have on water supplies.

Title: Trace Element and Major Component Balances Around the Synthane PDU Gasifier

Authors: A. J. Forney, W. P. Haynes, S. J. Gasior, R. M. Kornosky, C. E. Schmidt and A. G. Sharkey, Jr.

Performing Organization: Pittsburgh Energy Research Center, Pittsburgh, PA

Sponsoring Agency: U. S. Energy Research and Development Administration Pittsburgh, PA

Report No./Journal: PERC/TPR-75/1

NTIS/GPO No.: Unknown

Type of Report: Government Technical Progress Report, August, 1975

Abstract

This report presents the results from feed coal and non-gaseous products for 65 trace elements. A series of gasification tests was run in the Synthane PDU gasifier in order to define the distribution of trace elements in the effluent streams that enter and leave the gasifier. Feed coal, filter fines, char, tar, and water effluents were analyzed.

Title: Fate of Trace Constituents of Coal During Gasification

Authors: A. Attari

Performing Organization: Institute of Gas Technology, I.I.T. Center,
3424 South State Street, Chicago, IL 60616

Sponsoring Agency: EPA, Office of Research and Development, NERC, RTP
Control Systems Laboratory, Research Triangle Park,
NC

Reprot No./Journal: EPA-650/2-73-004

NTIS/GPO No.: PB-223-001 **Type of Report:** Final Technical

Abstract

Results of an investigation of the fate of trace elements in coal during the Hygas coal gasification process is presented. The work is from a six month study to set up laboratory analytical methods to analyze for Sb, As, Be, Cd, Cr, Pb, Hg, Ni, Se, Te, and V. The samples analyzed were representative of the coal input and the solid effluent of the pretreatment hydrogasification and electrothermal stages of the IGT pilot plant. The data indicated that a substantial amount of some of these elements was removed from coal during the gasification process.

Analysis of the elements was performed with a Perkin-Elmer Model 303 double beam atomic absorption spectrophotometer with a background compensator installed internally, a nebulizer burner assembly, and a Sargent TR 10" strip chart recorder. An international plasma low temperature asher [(LTA) IPC Model 1005B] was used for ashing the coal. Sample workup prior to atomic absorption analysis consisted of acid dissolution of coal ash using a perchloric-hydrofluoric acid technique.

Mercury analysis could not be conducted in this manner since losses were encountered. Mercury was determined by vapor phase analysis via gold amalgamation.

The gasification experiment utilized Pittsburgh No. 8 Seam bituminous coal.

Title: Characterization of Mineral Matter in Coals and Coal Liquefaction Residues

Authors: P. L. Walker, Jr., W. Spackman, P. H. Given, E. W. White, A. Davis, R. G. Jenkins

Performing Organization: Coal Research Section, College of Earth and Mineral Sciences, Pennsylvania State University, University Park, PA

Sponsoring Agency: Electric Power Research Institute, 3412 Hillview Ave., Palo Alto, CA 94304

Report No./Journal: EPRI 366-1, December, 1975

NTIS/GPO No.: Unknown **Type of Report:** Publication

Abstract

This is the first of the annual reports for a program which began January 1, 1975 and is scheduled to run through December 31, 1977. The mineral matter in American coal and the residues resulting from their hydrogenative liquefaction were described. The characterization techniques which were employed during the first year of this program were reflectance of organic and inorganic fractions in incident light, light microscopy, computer evaluation of scanning electron microscope images, infra-red spectroscopy, x-ray diffraction, sedimentation, surface areas from gas adsorption, helium densities, magnetic measurements and transmission electron microscopy.

Samples of feed coals and liquefaction residues were supplied by H. R. I., Southern Servies, Universal Oil, Lummus Co. and Pittsburgh and Midway Coal Mining Co. The techniques employed the polishing of a section of coal which was subsequently analyzed by optical and electron microscopic techniques. The analyses for minerals were performed

on these polished sections by a combination of techniques (ARM and CESEMI). Low-temperature ash was prepared from representative samples of coal and residues and then subjected to analysis by x-ray diffrection, infra-red spectroscopy and spectro-chemical analysis. Thus qualitative and quantitative analyses for the major minerals were obtained.

Title: Trace Element and Major Component Balances Around the Synthane PDU Gasifier

Authors: A. J. Forney, W. P. Haynes, S. J. Gasior, R. M. Kornosky, C. E. Schmidt and A. G. Sharkey

Performing Organization: Pittsburgh Energy Research Center, Pittsburgh, PA

Sponsoring Agency: U. S. ERDA, Washington, DC

Report No./Journal: PERC/TPR-75/1

NTIS/GPO No.: Unknown Type of Report: Government Publication

Abstract

A series of gasification tests was run in the Synthane PDU gasifier in order to define the distribution in the effluent streams of trace elements in the coals that enter the gasifier. The feed coal and non-gaseous products were analysed for 65 trace elements. Most of the elements were found in the char and dust with some also in the tars and waters. The report also indicates some problems with the availability of accurate methods of analysis ot make reasonable balances of the trace elements.

The trace element analysis was done on coal feed, feed water, char, fines, tar, water and gases derived from Illinois No. 6 coal using the technique of spark-source mass spectrometric analysis. Trace elements in the gas phase were also determined by neutron activation. Mercury analysis was performed by flameless atomic absorption procedures.

Title: Characterization of the Resin Fraction from Various Low Temperature Tar Pitches

Authors: C. Karr, Jr. and J. R. Comberiati

Performing Organization: Low-Temperature Tar Unit, Morgantown Coal Research Center, Morgantown, WV

Sponsoring Agency: Bureau of Mines: U. S. Department of Interior

Report No./Journal: Bulletin 636, Bureau of Mines

NTIS/GPO No.: Unknown Type of Report: Project Report

Abstract

Resins from a bituminous pitch, a bituminous coal, a lignite tar, a sub-bituminous pitch, and an electrode binder pitch were investigated. The compositions of each of these resins were determined by four independent methods of structural determination: (1) molecular formula and ring analysis, including ring arrangemnt; (2) infra-red and ultra-violet spectra; (3) combined pyrolysis/gas chromatography; and (4) catalytic dehydrogenation followed by spectral and pyrolytic analysis. The approximate formula $C_{28}H_{24}O_2$ was assigned to a benzene-soluble, petroleum ether-insoluble resin (molecular weight 395) from a low-temperature pitch. It is suggested that an average compound with about seven rings, not of which all were aromatic, could account for this formula.

Ring analysis, including the determination of ring arrangement, showed that the high molecular weight resins had a picene- or benzopicene-type skeleton with four or five aromatic rings, one or two saturated rings, five to ten methyl grups, and two to four oxygen atoms/molecule. The major substituents were phenolic hydroxyl and methyl groups. Carbonyl groups were present, conjugated with either aromatic rings, olefinic groups, or both.

Title: Comparison of Pitch Resins from Different Sources by Combined
Pyrolysis and Gas-Liquid Chromatography

Authors: C. Karr, J. R. Comberiati and W. C. Warner

Performing Organization: Morgantown Coal Research Center, Morgantown,
West Virginia

Sponsoring Agency: Bureau of Mines, U. S. Department Interior, Morgantown,
West Virginia

Report No./Journal: Anal. Chem., 35, 441 (1963)

NTIS/GPO No.: NA Type of Report: Publication

Abstract

The technique of combined pyrolysis and gas-liquid chromatography was used for comparison of various pitch resins derived from a low-temperature Texas lignite tar, a low-temperature nugget Wyoming sub-bituminous coal tar, a low-temperature West Virginia bituminous coal tar and an electrode binder pitch from a high temperature coke oven bituminous tar. The low-temperature tars were prepared in a fluidized bed carbonization at about 500°C. Analysis was performed on benzene-soluble and petroleum ether-insoluble, resins isolated from these sources.

This report indicates that the yield of total liquid products from about C_5-hydrocarbons through the cresols decreased as the coal rank decreased and also, in the case of bituminous coal, as the carbonization temperature was increased. The percentage of aromatics in the products (of pyrolysis) increased in going from sub-bituminous to bituminous to coke oven material but the highest yield of aromatics was obtained from the lignite resin. Phenols were observed in the pyrolysis products from all of the resins. However, the lignite resin was the only one that yielded phenols in significant amounts. According to these authors,

this result is in line with the observation that lignite tar has a much higher proportion of phenols than other tars. Quantitation was also performed for the pyrolysis products from the four different resins. In general, ~20 pyrolysis products were observed. These were primarily branched-chain alkanes and alkenes, aromatics such as ethylbenzene and the xylenes, phenol and the cresols.

Title: Molecular Profile Analysis of Coal Products

Author: M. Anbar

performing Organization: Stanford Research Institute, Mass Spectrometry
Research Center, Menlo Park, CA 94025

Sponsoring Agency: Electric Power Research Institute, 3412 Hillview
Ave., Palo Alto, CA 94304

Report No./Journal: EPRI 316-1

NTIS/GPO No.: PB-248 962 Type of Report: Final Report,
October, 1975

Abstract

The objectives of this research program were to develop instrumentation and experimental methodology for characterizing coal liquefaction products by mass spectrometric techniques. The feasibility of analyzing coal liquefaction by field ionization mass spectrometry was examined and confirmed. Under this program was developed: (1) a novel field ionization source that can handle non-volatile materials and (2) computerized data handling techniques to generate noise-free spectra.

The coal liquefaction products wre produced either by solvent refinement or catalytic hydrogenation of coal. The compounds produced were a complex mixture of organic compounds which included aliphatic and aromatic hydrocarbons, phenolics and basic heterocyclic compounds. The diverse compounds observed had molecular weights ranging from 100 to a few 1,000 and included highly volatile materials like benzene as well as materials of extremely low volaility like the asphaltenes. The analysis was primarily conducted on a 90° sector magnetic mass spectrometer equipped with a field ionization source developed under another project at this research facility.

Title: Compositional Analysis of Synthoil from West Virginia Coal

Authors: P. W. Woodward, J. G. Stuerm, Jr., J. W. Vogh, S. A. Holmes,
and J. E. Dooley

Performing Organization: Bartlettsville Energy Research Center, Bartlettsville, Oklahoma

Sponsoring Agency: U. S. ERDA, Washington, DC

Report No./Journal: PERC/RI-76/2, January, 1976

NTIS/GPO No.: Unknown Type of Report: Government Document

Abstract

This report describes a synthetic crude oil (Synthoil) derived from West Virginia Pittsburgh seam coal by the Synthoil process which was separated into three distillates an a residual fraction. The distillate fraction (<207°C) was further separated and characterized by gas chromatography and spectral techniques. The 207-363°C and 363-531° boiling distillates were further separated and characterized by methods developed by the Bureau of Mines for characterization of the heavy end of petroleum. Each of the higher boiling distillates was separated by dual packed column absorption chromatography into four concentrates: saturates, monoaromatics, disromatics and polyaromatic polar. The saturated compounds were characterized directly by mass spectromety. Both the monoaromatic and diaromatics concentrates were further separated by gel permeation chromatography (gpc) before characterization by gc/mass spectral correlations and nuclear magnetic resonance spectrometry. Acids and bases were extracted from the polyaromatic polar concentrates before gpc separation and mass spectral analysis. A composite semi-quantitative analysis of the distillate fractions for the saturates,

monaromatics, diaromatics, polyaromatics and other compounds was conducted.

The monoaromatics accounted for about 27% of the 207-363°C distillate and only 5% of the 363-531°C distillate. These compounds consisted of alkylbenzenes and the naphthalenologs thereof with up to 6 naphthalene rings on the benzene nucleus. The average carbon number of this distillate was C_{13} with an average range of C_{10} to C_{28}, compared with an average carbon number of C_{22} and an average range of C_{15} to C_{30} for the 363-531° distillate. High resolution mass spectral data were used to verify the monoaromatic characterizations.

Diaromatics accounted for about 22% of both distillates. Diaromatic types in the 207-363°C distillate corresponded to naphthalenes and /or diphenyl alkanes and their naphthalenologs with an average carbon number of C_{13} and an average range of C_{10}-C_{26}. High resolution mass spectral data were obtained along with nmr and fluroescence data to verify the diaromatic characterizations.

The acid and base extraction of the 207-363°C polyaromatic polar consisted of four fractions. These were hydrocarbon neutrals, weak acids, strong acids and bases amounting to 10.3, 7.2, 9.1 and 3.4%, respectively, of the distillate. The hydrocarbon fraction including some neutral heteroatomic types was further separated by gpc and analyzed by mass spectral techniques. The major compound types corresponded to azanaphthalenes, phenanthrenes and anthracenes and their naphthalenologs. Other hydrocarbon types found were: diazanaphthalenes, pyrenes, benzopyrenes, perylenes, chrysenes and their naphthalenologs. Nitrogen compounds were also detected by high resolution mass spectrometry in the hydrocarbon fraction of the 207-363°C polyaromatic polar concentrate.

These consisted of pyridans, indoles, carbazoles and acridines and amounted to only about 7.8% of the hydrocarbon fraction. Oxygenated compounds were predominantly dibenzofurans.

Title: Identification of Distillable Paraffins, Olefins, Aromatic Hydrocarbons, and Neutral Heterocyclics from a Low-Temperature Bituminous Coal Tar

Authors: C. Karr, Jr., P. A. Estep, T. C. L. Chang and J. R. Comberiati

Performing Organization: Morgantown Energy Research Center, Morgantown, WV

Sponsoring Agency: Bureau of Mines, U. S. Dept. of Interior, Morgantown, WV

NITS/GPO No.: Unknown Type of Report: Government Document

Abstract

This report presents the extensive characterization which was conducted on neutral oil components in a low-temperature bituminous coal tar. A total of 133 individual compounds was identified with respect to individual isomers and at least 55 other compounds were indicated to be present. The amounts were determined in all instances. Detailed descriptions are presented for the separation and qualitative and quantative characterization of neutral oil components. The techniques primarily used were: micro-vacuum fractional distillation, displacement, liquid chromatography, gas-liquid chromatography, countercurrent distribution and infra-red and ultra-violet spectrophotometry.

The report also describes the synthesis of authentic standards of alkylindenes. The ultra-violet and infra-red spectra of 134 polycyclic compounds ranging from alkylindene to alkylphenanthrenes either found in the distillable neutral oil or though likely to be present are also given.

Title: Gas-Liquid Chromtographic Analysis of Aromatic Hydrocarbons
Boiling Up To 218° in a Low-Temperature Coal Tar

Authors: T. C. L. Chang and C. Karr, Jr.

Performing Organization: Low-Temperature Tar Laboratory, Morgantown Coal Research Center, Morgantown, WV

Sponsoring Agency: Bureau of Mines, U. S. Dept. Interior, Morgantown, WV

Report No./Journal: Analytica Chimica Acta, 21, 474 (1959)

NTIS/GPO No.: NA Type of Report: Publication

Abstract

This paper describes the results of analysis for aromatic hydrocarbons boiling upto 218° which are present in the neutral oil portion of a low-temperature bituminous coal tar. In this work, gas-liquid chromatography and other modern analytical techniques were used for analysis. Fifty-two aromatic hydrocarbons boiling upto 218° were found and their quantities were determined. Besides indanes, benzofurans and indenes, the aromatic hydrocarbons identified were methylated, ethylated or propylated benzenes. No butylbenzenes have been found in this particular tar. A linear relationship between log of relative retention time and normal boiling point was demonstrated for C_8, C_9, C_{10}, C_{11} and C_{12} alkylbenzenes which lie on five parallel lines whose separation from each other is related to the logarithm of the number of carbon atoms in the alkyl group.

Title: A Note on Determining the Arrangement of Rings in Polynuclear Aromatic Compounds of Coal Tar Pitch Fractions

Author: C. Karr, Jr.

Performing Organization: Low-Temperature Tar Laboratory, Morgantown Coal Research Center, Morgantown, WV

Sponsoring Agency: Bureau of Mines, U. S. Dept. Interior, Morgantown, WV

Report No./Journal: Fuel, 39, 119 (1960)

NTIS/GPO No.: NA Type of Report: Publication

Abstract

This publication describes a mathematical treatment of ring index (total rings/carbon atom, R/C) vs. atomic hydrogen to carbon ratio (H/C) for several common series of condensed polynuclear aromatic compounds. The method demonstrates that each series has a different set of expressions of R/C and H/C in terms of R from which the arrangement of rings can be differentiated for compounds containing less than 10 rings.

Title: Extracting Neutral Low-Temperature Lignite Tar Fractions with Dipropionitrile Solvents

Authors: P. L. Campbell and J. M. Stuckey

Performing Organization: Morgantown Energy Research Center, Morgantown, WV

Sponsoring Agency: Bureau of Mines, U. S. Dept. of Interior, Morgantown, WV

Report No./Journal: RI-5742 (1961)

NTIS/GPO No.: Unknown Type of Report: Government Document

Abstract

This report presented the investigations on methods of upgrading tar obtained by low-temperature carbonization of lignite. Several solvents such as β,β'-oxydipropionitrile, β,β'-iminodipropionitrile, and β,β'-thiodipropionitrile were found to be effective solvents for extracting aromatics (aromatic hydrocarbons plus polar compounds) from coal tar neutral distillate fractions. Batch extractions show that these solvents extracted approximately the same percentage of aromatics from various neutral oil fractions boiling between ~170-350°C. Continous countercurrent extractions were used in conjunction with these solvents. Other solvent partitioning methodology is also presented in this report for extracting the neutral fraction or aromatic and polar hydrocarbons.

Title: Gas-Liquid Chromatographic Analysis of Aromatic Hydrocarbons
Boiling Between 202-280° in a Low-Temperature Coal Tar

Authors: T. C. L. Chang and C. Karr, Jr.

Performing Organization: Low-Temperature Tar Laboratory, Morgantown
Coal Research Center, Morgantown, WV

Sponsoring Agency: Bureau of Mines, U. S. Dept. Interior, Morgantown,
WV

Report No./Journal: Analytica Chimica Acta, 24 343 (1961)

NTIS/GPO No.: NA Type of Report: Publication

Abstract

This study utilized gas-liquid chromatography in conjunction with infra-red and ultra-violet spectrophotometry to analyze aromatic hydrocarbons boiling between 202-280°C in the neutral oil portion of a low-temperature bituminous coal tar. A total of 48 compounds was identified of which 20 were alkylnapthalenes. Of these compounds, nine had also been mentioned in a previous report. Quantitative determinations were made on nearly all of the components. This analysis is by far the most detailed one carried out up to this year for the alkylnaphthalene cut of a low-temperature coal tar. In this report, the alkylnaphthalenes with equal numbers of carbon atoms and their alkyl groups were demonstrated to display a linear relationship between log relative retention and normal boiling point, a situation which is similar to that for the alkylbenzene series described in another report. The values for the C_{11}, C_{12}, C_{13} alkylnaphthalenes lie on three parallel lines.

Title: Properties of Compounds in Coal Carbonization Products

Authors: H. C. Anderson and W. R. K. Wu

Performing Organization: Pittsburgh Coal Research Center, Pittsburgh, PA

Sponsoring Agency: Bureau of Mines, U. S. Dept. Interior, Pittsburgh, PA

Report No./Journal: Bulletin 606, Bureau of Mines

NTIS/GPO No.: Unknown Type of Report: Government Document

Abstract

This compendium gives data for 832 compounds that have been found in the products of coal carbonization. Data for each compound include values found in the literature for frequently used properties as well as molecular folmula, structural formula, source, investigator and molecular weight. For example, the source of cyclohexene is listed as high temperature tar, Ref. 10-1360, bituminous low-temperature, Ref. 1140 and crude benzole boiling, 79-81.5°, Ref. 4-A4. Furthermore, 32 inorganic structural formulas and sources are tabulated.

The compendium is current to February of 1962.

Title: Ring Analysis and Spectral Characterization of Resins from Pitch
of Low-Temperature Tar

Authors: C. Karr, Jr., J. R. Comberiati and P. A. Estep

Performing Organization: Low-Temperature Tar Laboratory, Morgantown
Coal Research Center, Morgantown, WV

Sponsoring Agency: Bureau of Mines, U. S. Dept. Interior, Morgantown,
WV

Report No./Journal: Fuel, 41, 167 (1962)

NTIS/GPO No.: NA Type of Report: Publication

Abstract

This publication describes the analysis of resins from pitch of lignite, sub-bituminous and bituminous low-temperature tars by ring analysis and infra-red and ultra-violet spectrophotometry. The composition of the resins was primarily found to be aromatic compounds all having 4 or 5 aromatic rings/molecule. Saturated rings possible including ether groups were also determined to be present and fused into the hydrocarbon skeleton. The lower molecular weight resins have a linear arrangement of rings with 1 or 2 saturated rings in addition to the aromatic rings. According to this report, the higher molecular weight resins apparently have a globular or compact arrangement of rings with 5-7 saturated rings in addition to the aromatic rings. The resins were found to have 2-6 oxygen atoms/molecule. Phenolic hydroxyl groups were also present and probably accounted for the majority of the oxygen. Carbonyl groups were conjugated with either aromatic rings of olefinic groups or both. Most of the aromatic rings were found to have at least 2 substituents. These were mostly either methyl groups or fused saturated rings or both. Alkyl substitution was greater for the lower molecular weight resins.

Title: Estimation of Ratio of Isomers in Coal Tar from Free Valence Numbers

Author: C. Karr, Jr.

Performing Organization: Morgantown Coal Research Center, Morgantown, WV

Sponsoring Agency: Bureau of Mines, U. S. Dept. Interior, Morgantown, WV

Report No./Journal: Fuel, 41 299 (1962)

NTIS/GPO NO.: NA   Type of Report: Publication

Abstract

The substance of this article is that a relationship exists between the divergence in the distribution of isomers in low-temperature coal tars and the predicted thermodynamic equilibrium distributions in the kinetic distribution at 500°C for coal structure and tar composition. The ratio of isomers in the kinetic distribution was estimated from the free valence numbers assuming a free radical mechanism of alkylation. The purpose thus is to predict the composition of the tar which is derived during the low-temperature carbonization process.

Title: Gas-Liquid Chromatographic Analysis of C_{10}-C_{16} n-Paraffins, Iso-Parafffins an α-Olefins in a Low-Temperature Coal Tar

Authors: T. C. L. Chang and C. Karr, Jr.

Performing Organization: Low-Temperature Tar Research, Morgantown Coal Research Center, Morgantown, WV

Sponsoring Agency: Bureau of Mines, U. S. Dept. Interior, Morgantown, WV

Report No./Journal: Anal. Chimica Acta, 26, 410 (1962)

NTIS/GPO No.: NA Type or Report: Publication

Abstract

In this report, 21 C10-C16 hydrocarbons, seven each of n-paraffins, 2-methylalkanes and α-olefins were identified in a low-temperature bitimunous coal tar by means of gas-liquid chromatography. Quantitative determinations were made on all of these constituents. The study found that curves for the plots of the logarithm or relative retention time against normal boiling points for C_{10}-C_{16} n-paraffins and α-olefins were parallel. A similar parallel curve for the 2-methylalkane series was derived using the known point of 2-methyldecane. This correlation curve was used for the identification of several 2-methylalkanes. Naphthenes and trans-olefins were found in small amounts.

Title: Structure Determination of Resins from Pitch of Low-Temperature
Tar by Combined Pyrolysis and Gas-Liquid Chromatography

Authors: C. Karr, Jr., J. R. Comberiati and P. A. Estep

Performing Organization: Low-Temperature Tar Laboratory , Morgantown,
Coal Research Center, Morgantown, WV

Sponsoring Agency: Bureau of Mines, U. S. Dept. Interior, Morgantown,
WV

Report No./Journal: Fuel, 42, 211 (1963)

NTIS/GPO No.: NA Type of Report: Publication

Abstract

Sub-bituminous coal tar resin which had been heated for several seconds at a temperaure of 528° was subjected to pyrolysis followd by gas-liqud chromatography. The major pyrolysis products were 2,3,4-trimethylpentane, 2,2,4-trimethylpentane and benzene in decreasing quantity, respectively. Toluene and the 3 xylenes were also present, but no higher-boiling volatile products were detected. The conclusion these authors give is that this resin is made up largely of isolated benzene rings joined together by saturated fused multi-ring systems with saturated bridged carbons including quaternary carbons.

Title: Composition of Pyridine Extracts from Reduced and Untreated
Coals as Determined by High Resolution Mass Spectrometry

Authors: T. Kessler, R. Raymond and A. G. Sharkey, Jr.

Performing Organization: Pittsburgh Coal Research Center, Pittsburgh, PA

Sponsoring Agency: Bureau of Mines, U. S. Dept. of Interior, Pittsburgh, PA

Report No./Journal: Fuel, 48 179 (1964)

NTIS/GPO No.: NA Type of Report: Publication

Abstract

High resolution mass spectrometric analysis was performed on the volatile portion of pyridine extracts obtained from reduced an untreated vitarin. This process demonstrated the following: (1) a greater concentration of oxygen-containing compounds in the reduced vitrain compared with that in the untreated vitrain; (2) an approximate eight-fold decrease in the organic sulfur compounds in the vitrain following reduction which was thought to be consistent with the decrease in sulfur as shown by ultimate analysis; (3) a lower concentration of higher molecular weight hydrocarbons such as 3-ring aromatics in the reduced vitrain; and (4) a significant increase in the amount of hydroaromatic compounds in the reduced vitrain.

The reduced sample was prepared by reacting vitrain from Pittsburgh seam HVAB coal with lithium-ethylenediamine.

Title: Composition of Pyridine Extracts from Reduced and Untreated
Coals as Determined by High Resolution Mass Spectrometry

Authors: T. Kessler, R. Raymond and A. G. Sharkey, Jr.

Performing Organization: Pittsburgh Coal Research Center, Pittsburgh, PA

Sponsoring Agency: Bureau of Mines, U. S. Dept. of Interior, Pittsburgh, PA

Report No./Journal: Fuel, 48, 179 (1964)

NTIS/GPO No.: NA   Type of Report: Publication

Abstract

High resolution mass spectrometric analysis was performed on the volatile portion of pyridine extracts obtained from reduced an untreated vitrain. This process demonstrated the following: (1) a greater concentration of oxygen-containing compounds in the reduced vitrain compared with that in the untreated vitrain; (2) an approximate eight-fold decrease in the organic sulfur compounds in the vitrain following reduction which was thought to be consistent with the decrease in sulfur as shown by ultimate analysis; (3) a lower concentration of higher molecular weight hydrocarbons such as 3-ring aromatics in the reduced vitrain; and (4) as significant increase in the amount of hydroaromatic compounds in the reduced vitrain.

The reduced sample was prepared by reacting vitrain from Pittsburgh seam HVAB coal with lithium-ethylenediamine.

Title: Quantitative Infra-red Microanalysis of High Boiling Aliphatic
Neutral Oil Fractions

Authors: P. A. Estep and C. Karr, Jr.

Performing Organization: Morgantown Coal Reseach Center, Morgantown, WV

Sponsoring Agency: U. S. Bureau of Mines, Dept. of Interior, Morgantown, WV

Report No./Journal: Anal. Chem., 36, 2115 (1964)

NTIS/GPO No.: NA Type or Report: Publication

Abstract

This report discussses a quantitative infra-red microanalytical procedure that has been developed for characterizing neutral oils from low-temperature coal tars. The neutral oil distillate fractions analyzed in this work were obtained from a low-temperature bituminous coal tar which had been isolated by countercurrent distribution in a dual solvent system of iso-octane and 90% by weight ethanol and water. The alphatic material was recovered from the upper phase solvent (iso-octane) in the automatic fraction collector of a Craig countercurrent distribution (CCD) apparatus. The lower phase contained primarily the aromatics. A variety of both saturated and olefin types in the C_{15}-C_{20} range inclusive was identified in these samples. The primary technique of molar absorptivity in the uv wavelenghts and infra-red spectroscopy was used for identifying n-alkanes, methylalkanes, α-olefins, and branched α-olefins.

Title: Analysis of Aromatic Hydrocarbons from Pitch Oils by Liquid Chromatography on Gas Chromatography Analog

Authors: C. Karr, Jr., E. E. Childers, W. C. Warner and P. E. Estep

Performing Organization: Morgantown Coal Research Center, Morgantown, WV

Sponsoring Agency: Bureau of Mines, U. S. Dept. Interior, Morgantown, WV

Report No./Journal: Anal. Chem., 36, 2105 (1964)

NTIS/GPO No.: NA Type of Report: Publication

Abstract

This paper describes the technique of liquid chromatography on the gas chromatography analog for analyzing complex natural mixtures of high boiling aromatic hydrocarbons including the identification of individual constitutents. Pitch oil fractions boiling in the range from 290-315°C were analyzed by this method and shown to contain about 70 components. However, only 11 of these were readily identified by relative retentions and by infrared and ultra-violet spectrophotometry. Compounds identified were: dibenzofuran, fluroene and various methyl derivatives and phenanthrene. The pitch oils were derived from a low-temperature bituminous coal tar. They were obtained by distillation in a spinning band column with a head pressure of about 0.015 mm of mercury. The origin of the low-temperature bituminous coal tar was not described.

Title: Countercurrent Distribution of High Boiling Phenols from a
Low-Temperature Coal Tar

Authors: C. Karr, Jr., P. A. Estep and L. L. Hirst, Jr.

Performing Organization: Low Temperature Tar Laboratory, Morgantown,
Coal Research Center, Morgantown, WV

Sponsoring Agency: Bureau of Mines, U. S. Dept. of Interior, Morgantown,
WV

Report No./Journal: Anal. Chem., 32, 463 (1960)

NTIS/GPO No.: NA Type of Report: Publication

Abstract

This publication describes the method of countercurrent distribution for isolation of tar acids in complex mixtures of high boiling phenols. Tar acids boiling at 231-331° from a low-temperature bituminous coal tar were fractionated and analyzed. The presence of 84 individual compounds was demonstrated: 24 were identifed with respect to specific isomers and 36 with respect to structural type, the remainder being tar acids of unknown structure. Quantification of all components was performed.

Title: Structure Determination of Pitch Resin by Catalytic Dehyrdogenation

Authors: C. Karr, Jr., K. B. McCaskill and J. J. Kovach

Performing Organization: Low-Temperature Tar Laboratory, Morgantown Coal Research Center, Morgantown, WV

Sponsoring Agency: Bureau of Mines, U. S. Dept. of Interior, Morgantown, WV

Report No./Journal: Fuel, 44, 437 (1965)

NTIS/GPO No.: NA Type of Report: Publication

Abstract

A structure determination of the benzene soluble, ethyl ether-insoluble pitch resin from a low-temperature bituminous coal tar was made by catalytic dehydrogenation if four different pure solvents with subsequent examination by infrared and ultra-violet spectrophotometry. Analaysis of the structural features indicated that the original resin contained alcoholic OH groups of a type which could be readily converted to ketone groups of the anthrone or quinone kind by dehydrogenation and naphthalenic rings partially substituted with OH and methyl groups which were attached to aromatic rings with a considerably higher degree of substitution. The dehydrogenation of the naphthalenic rings yielded a great increase in three or four adjacent hydrogens on aromatic rings compared to one and two hydrogens.

Title: Mass Spectra of Pyrolyzates of Several Aromatic Structures
Identified in Coal Extracts

Authors: A. G. Sharkey, Jr., J. L. Schultz and R. A. Friedel

Performing Organization: Pittsburgh Coal Research Center, Pittsburgh, PA

Sponsoring Agency: Bureau of Mines, U. S. Dept. of Interior, Pittsburgh, PA

Report No./Journal: Carbon, 4, 365 (1966)

NTIS/GPO No.: NA Type of Report: Publication

Abstract

This publication presented the mass spectra of products from the liquid phase pyrolysis of 20 hydrocarbons having 1-4 aromatic rings and molecular weights from 116 (indene) to 228 (chrysene). The pyrolyzates of several structural types were found in the material extracted from Pittsburgh seam (HVAB) coal with pyridine at room temperature. The highest mass spectral peaks of the pyrolyzates of naphthalenes, phenanthrenes and pyridines were 254, 354, and 402, respectively, corresponding to dehydrative dimers of these compounds. The mass spectrometric and other data indicated that the major components of the liquid and solid products from a low-temperature carbonization of coal have molecular weights below 400.

Title: Liquid Fuels from Tars by Carbonization of Coal in Hydrogen Atmospheres

Authors: C. Karr, Jr., J. O. Mapstone, Jr., L. R. little, Jr., R. E. Lynch and J. R. Comberiati

Performing Organization: Morgantown Energy Research Center, Morgantown, WV

Sponsoring Agency: Bureau of Mines, U. S. Dept. of Interior, Morgantown, WV

Report No./Journal: I & EC Product Research and Development, 10, 204 (1971)

NTIS/GPO NO.: NA Type of Report: Publication

Abstract

This study was on the yield and quality of gasoline, with the boiling range of light oil obtained by fixed-bed carbonization of coal around 950°F in hydrogen atmospheres. The total quantities of aliphatics, benzene, xylenes and toluenes were estimated under various reactor conditions. The techniques employed for their analysis did not distinguish the individual components.

Title: High Resolution Mass Spectrometric Investigation of Heteroatom
Species in Coal Carbonization Products

Authors: J. L. Shultz, T. Kessler, R. A. Friedel and A. G. Sharkey, Jr.

Performing Organization: Pittsburgh Energy Research Center, Pittsburgh, PA

Sponsoring Agency: Bureau of Mines, U. S. Dept. of Interior, Pittsburgh, PA

Report No./Journal: Fuel, 51, 242 (1972)

NTIS/GPO No.: NA

Type of Report: Publication

Abstract

High resolution mass spectrometry was used to determine the organic species present in coal carbonization products, airborne particulates and municipal effluents. Qualitative analysis of a 80-85°C softening point pitch yielded molecular formulas for 239 compounds, which corresponded to a minimum of 108 structural types, and their alkyl derivatives. Of these, 76 structural types were composed of eight different combinations of elements: structures containing carbon-hydrogen, carbon-hydrogen-oxygen, and carbon-hydrogen-nitrogen were the most numerous while species containing S, N_2, ON, O_2 and O_2N_2 were also observed.

Title: Identification and Determination of 1,4-Benzoquininone in Waste
Waters from the Coal Processing Industry

Author: H. Thielemann

Performing Organization: Unknown

Sponsoring Agency: German Government

Report No./Journal: Z. Wasser-Abwasser-Forschung, 7, 91 (1974)

NTIS/GPo No.: NA Type of Report: Publication

Abstract

This study presents the determination of phenolic compounds in waste waters from the coal working industry. An non-biodegradable and toxic substance (1,4-benzoquinone) in waste waters from the coal processing industry was detected by thin-layer chromatography utilizing specific spray reagents. These reagents were: 4-aminoantipyrine, rhodamine-B and uv, 2,6-dibromoquinonechloroamide, phosphomolybdic acid, iodine localization and 1N sodium hydroxide.

Title: Analysis of Polycylic Organic Material in Coal, Coal Ash, Fly Ash and Other Fuel and Emission Samples

Authors: A. G. Scharkey, J. L. Schultz, C. White and R. Lett

Performing Organization: U. S. Energy Research and Development Administration, Pittsburgh Energy Research Center, Pittsburgh, PA

Sponsoring Agency: EPA, Office of Research and Development, Industrial Environmental Research Laboratory, Research Triangle Park, NC

Report No./Journal: EPA-600/2-76-075

NTIS/GPO No.: PB-253-453 Type of Report: Government Document

Abstract

This report describes the investigation of the major polynuclear aromatic hydrocarbons in samples derived from various fuel conversion processes and related planned emissions utilizing the technique of high resolution mass spectrometry. The particulate materials and extracts of hydrocarbons studied in the particulate materials were collected on filters placed in flue gas streams from coking, smelting and similar industrial operations.

Title: Gas-Liquid Chromatography of Some Alkyl Phenols

Authors: P. M. Brown

Performing Organization: West Virginia University

Sponsoring Agency: West Virginia University

Report No./Journal: Master of Science Thesis, West Virginia University

NTIS/GPO No.: none Type of Report: MS Thesis, 1957

Abstract

Low boiling phenols in low-temperature coal tar were identified and quantiated using the technique of glc in conjunction with infrared spectroscopy. Eighteen compounds were identfied among which were phenol, 3 methylphenols, 3 ethylphenols, 6 dimethylphenols, trimethylphenol and ethylmethylphenol. The coal used to prepare the low-temperature tar was mined by the Pittsburgh Consolidated Coal Co. The tar was prepared in a low temperature (480-510°C) fluidized bed carbonization pilot plant at Library, PA. The tar was deashed to remove solids and dehydrated by flashing at 175°C to remove water and other volatiles. Thus many of the volatile organic compounds as well as organometallic substances were not analyzed by this procedure. The procedure for stripping the volatile constituents consisted of a rotary vacuum stripper operated at 0.1 mm pressure and 110-125°C. Thus only the semi-volatile organics were condensed by the water condenser. The highly volatile organic fraction was not recovered by this procedure.

The highest concentration was 25% by weight of 2-methylphenol followed by 22.5% of phenol. 3-Methylphenol and 2,4-dimethylphenol were 13% by weight in the tar examined.

Title: Physical Properties of Low Boiling Phenols, A Literature Survey

Author: C. Karr, Jr.

Performing Organization: Morgantown Research Center, Morgantown, WV

Sponsoring Agency: Bureau of Mines, U. S. Dept. of Interior, Morgantown, WV

Report No./Journal: Information Circular 7802, September, 1957

NTIS/GPO No.: Unknown Type or Report: Government Document

Abstract

This report contains a comprehensive survey on the physical properties of 183 different phenols boiling below 260°C. These include phenols with various combinations of methyl, ethyl, propyl and butyl groups as well as a few indanols and catechols.

Title: Analysis of Low-Temperature Tar Phenols Boiling Up to 234°C

Authors: C. Karr, Jr., P. N. Brown, P. A. Estep and G. L. Humphrey

Performing Organization: Low-Temperature Tar Laboratory, Morgantown
Coal Research Center, Morgantown, WV

Sponsoring Agency: Bureau of Mines, U. S. Dept. Interior, Morgantown,
WV

Report No./Journal: Fuel, 37 227 (1958)

NTIS/GPO No.: NA Type of Report: Publication

Abstract

In this publication, the low-temperature bituminous coal tar phenols boiling up to 234°C were identified and quantiated ty gas-liquid chromatography. Chromatographic fractions were collected for infrared analysis for the identification of phenols. The phenols were also determined by the conventional technique of fractional distillation followed by ir analysis. A comparison of the two independent techniques was made with a fairly good agreement obtained in the quantitative analysis of the bituminous coal tar phenols. Phenol, three cresols, six xylenols, three ethylphenols, 2 ethylmethylphenols and two trimethylphenols were analyzed.

The tar used in this work was made from a West Virginia bituminous coal in a fludized carbonization pilot plant at about 480-510°C. The raw tar was de-ashed, dehydrated and topped to about 175° at the plant. A Claisen alkaline extraction technique was used on both portions of the distillate with the phenols extracted from the low boiling portion representing about 0.08% of the tar. The phenols extracted from the main distillate represented 3.54 weight precent of the tar.

Title: Identification and Determination of Low Boiling Phenols in Low-Temperature Coal Tar

Authors: C. Karr, Jr., P. N. Brown, P. A. Estep and G. L. Humphrey

Performing Organization: Low-Temperature Tar Laboratory, Morgantown Coal Research Center, Morgantown, WV and Dept. of Chemistry, West Virginia University, Morgantown, WV

Sponsoring Agency: Bureau of Mines, U. S. Dept. of Interior, Morgantown, WV

Report No./Journal: Anal. Chem., 30, 1413 91958)

NTIS/GPO No.: NA   Type of Report: Publication

Abstract

This report describes the identification and quantitation by gas-liquid chromatography of the low boiling phenols in a low-temperature bituminous coal tar distillate. Phenols were also determined by the conventional technique of fractional distillation followed by infra-red analysis. A comparison of the two independent techniques was also made. Thirteen phenols were compared by these two techniques as to the estimated quantity (weight percent) given by each method. The agreement between weight percentages of phenols by infra-red and vapor-phase chromatographic analysis was within 1-3%.

Title: Extraction of Tar Acids with Aqueous Monoethyanolamine

Authors: Y. C. Chang and R. C. Johannsen

Performing Organization: Bureau of Mines, Morgantown, West Virginia

Sponsoring Agency: U. S. Dept. Of Interior, Morgantown, West Virginia

Report No./Journal: Journal of the Institute of Fuel, April, 174 (1959)

NTIS/GPO No.: NA Type of Report: Publication

Abstract

Research was performed on the examination of monoethanolamine as an effective extacting agent for tar acids from a coal-tar distillate derived from a sub-bituminous coal. It was concluded that this reagent improved the yield but decreased the quality as the concentration of monoethanolamine was changed from 30-70 volume percent and the concentration of the tar acid in the distillate was increased from 14-45%. The yields varied from 9-24 volume percent of the distillate and the neutral oil amounted to 5-40 volume percent of the extract.

The tar distillate used in this experiment was derived from a low-temperature tar supplied by the Denver Station of Federal Bureau of Mines. The parent coal was a sub-bituminous C coal of Smith Rowland bed, Wyodak mine, east of Gillette, Wyoming.

Other extraction procedures cited were aqueous methanol, an aqueous methanol and paraffinic hydrocarbon mixture and a glycerol and triethylene glycol mixture for the extraction of tar acids from coal tar distillates. This report suggests that monoethyanolamine used for the extraction of tar acids is superior to the alcoholic solvents; however, extraction with caustic soda is still the best suggested approach.

Title: Countercurrent Distribution of High Boiling Neutral Oils from Low-Temperature Coal Tar

Authors: P. A. Estep, C. Karr, Jr., W. C. Warner and E. E. Childers

Performing Organization: Morgantown Coal Research Center, Morgantown, WV

Sponsoring Agency: U. S. Bureau of Mines, Dept. of Interior, Morgantown, WV

Report No./Journal: Anal. Chem., 36, 1715 (1965)

NTIS/GPO No.: NA　　Type of Report: Publication

Abstract

This publication describes the method of countercurrent distribution for the analysis of complex mixtures of high boiling neutral oils. The neutral oil studied had boiling charcteristics at 275-344°C and was obtained from a low-temperature bituminous coal tar which had been fractionated by distillation and countercurrent distribution in a 60 tube apparatus. The upper phase used in the CCD was iso-octane, the lower phase was a 90 weight percent ethanol and water mixture. The contents of each tube were analyzed by infra-red and ultra-violet spectrophotometry. Fifty-one separate identifications were made, 19 for specific compounds. Quantification was also performed. The classes of compounds included aliphatics, naphthalenes, fluorenes, phenanthrenes, anthracenes, dibenzofurans and carbazoles.

Title: Evaluation of Low-Temperature Coal Tars by a Rapid Detailed Assay Based on Chromatography

Authors: C. Karr, Jr., J. R. Comberiati, K. B. McCaskill and P. A. Estep

Performing Organization: Low-Temperature Coal Tar Laboratory, Morgantown Coal Research Center, Morgantown, WV

Sponsoring Agency: Bureau of Mines, U. S. Dept. of Interior, Morgantown, WV

Report No./Journal: J. Appl. Chem., 16 22 (1966)

NTIS/GPO No.: NA Type of Report: Publication

Abstract

This paper describes a detailed assay based primarily on both liquid and gas chromatography which was developed for low-temperature coal tars. Using this assay, the lbs/ton of coal for various compounds of commerical interest could be determined by applying the information needed for an economic evalution of the tars in the carbonization processes. The amounts of approximately 100 individual compounds of several classes were determined including light oil components, tar acids and tar bases and neutral oil components such as naphthalenes and straight-chained paraffins, and olefins as well as the total amounts of these classes in the entire tar. Results for 6 different tars from the same coal are decribed.

Title: Ultraviolet Spectrophotometric Determination of Total Pyridines and Quinolines in Low-Temperature Coal Tar Distillates

Authors: T. C. L. Chang and C. Karr, Jr.

Performing Organization: Low-Temperature Tar Laboratory, Morgantown,
Coal Research Center, Morgantown, WV

Sponsoring Agency: Bureau of Mines, U. S. Dept. of Interior, Morgantown, WV

Report No./Journal: Bureau of Mines, U. S. Dept. of Interior, Morgantown, WV

NTIS/GPO No.: NA **Type of Report:** Publication

Abstract

This publication describes an ultraviolet spectrophotometric method for determining total pyridines and total quinolines in coal tar distillates. The procedure calls for extracting bases from the sample with acid and the extract is then adjusted to pH 12. The free bases are extracted from the alkaline solution with iso-octane. Ultra-violet spectra were obtained from the total quinolines and pyridines which were determined by using average absorbivities from pure compounds.

Title: Spectrophotmetric Determination of Small Quantities of Some
Individual Pyridine Bases by Successive Extractions

Authors: T. L. C. Chang and C. Karr, Jr.

Performing Organization: Low-Temperature Tar Laboratory, Morgantown,
Coal Research Center, Morgantown, WV

Sponsoring Agency: Bureau of Mines, U. S. Dept. of Interior, Morgantown, WV

Report No./Journal: Anal. Chem., 29, 1617 (1957)

NTIS/GPO No.: NA Type of Report: Publication

Abstract

A procedure is reported for determining small quantities of individual pyridine bases in aqueous methanol solutions based on the removal of methanol followed by two successive extractions with iso-octane. Concentrations of the bases in these two iso-octane extracts were determined by uv spectrophotometry. The distribution coefficient of the bases were also calculated. Based on the distribution coefficients of the total concentrations of the bases in the original samples, the estimated recoveries were about 90-100%. This method has been applied successfully to pyridine, α-picolene, 2,3-lutidine and quinoline. This paper is primarily concerned with the optimal conditions for the extraction of bases prior to the application of the methodology to low-temperature coal tar distillates.

Title: Spectrophotometric Analysis of the Distillable Low-Temperature Tar Bases

Authors: C. Karr, Jr. and T. C. L. Chang

Performing Organization: Bureau of Mines, Morgantown, WV

Sponsoring Agency: U. S. Dept. of Interior, Morgantown, WV

Report No./Journal: Journal of Institute of Fuel, December, 522(1958)

NTIS/GPO No.: NA Type of Report: Publication

Abstract

This report presents a detailed analysis of a typical low-temperature bituminous coal tar base mixture with a boiling point of up to about 355°C. The techniques employed were fractional vacuum distillation and spectrophotometric analysis. A total of 51 individual tar base compounds was identified in the tar base mixture and their quantities estimated. This work constitutes the first fairly comprehensive analysis of low-temperature bituminous coal tar bases since more than 80% of the compounds described had not been previously identified.

Infra-red and ultra-violet spectra of tar bases were the primary method of identification of the individual components. The tar examined by spectrometric methods used in this work was made from West Virginia, Pittsburgh-seam, high-volatile bituminous coal from a fluidized carbonization pilot plant operated at about 480-510°C. The raw tar was de-ashed, dehydrated and topped to about 175° at the plant. The pH of the acid extract containing the tar bases was adjusted to 12 with potassium hydroxide and the resulting mixture extracted with a 1 ℓ portion and three 500 ml portions of ether. The procedure essentially consisted of back extraction with acid for further purification and washing with aromatic solvents. The individual tar bases identified were

2,4-dimethylpyridine, 2,3-dimethylpyridine, 3,5-dimethylpyridine, 2,4,6-trimethylpyridine, 4-isopropylpyridine, 5-ethyl-2-methylpyridine, 4-ethyl-2-methylpyridine, 2,3-trimethylpridine, aniline, 2,6-dimethyl-4-ethylpyridine, N,N-dimethylaniline, 3-ethyl-4-methylpyridine, 2,3,5,6-tetramethylpyridine, 2,3-cyclopentenopyridine, 3-methylaniline, 2,3,4,6-tetramethylpyridine, N-methyl-2-methylaniline, 3,5-diethylpyridine (?), 2,5-dimethylaniline, 2-ethylaniline, 2,6-dimethylaniline, 3,5-dimethylaniline, quinoline, 2-methylquinoline, 8-methylquinoline, 2,8-dimethylquinoline, 7-methylquinoline, 6-methylquinoline, 4-methylquinoline, 2,7-dimethylquinoline, 2,4-dimethylquinoline, 2,6-dimethylquinoline, 2-phenylpyridine, 2,4,8-trimethylquinoline, 2,6,8-trimethylquinoline, 4,6-dimethylquinoline (?), 4-phenylpyridine, 2-methyl-6-phenylpyridine (?), 2,4,7-trimethylquinoline, 2,4,6-trimethylquinoline, 3,4-dimethylquinoline (?), 2-naphthylamine, N-benyl-2-methylaniline, N-benzyl-4-methylaniline, benzo[h]quinoline (7,8-benzoquinoline), acridine, phenanthridine, benzo[f]quinoline, 2,4-dimethylbenzo[h]quinoline (?), 2,4-dimethybenzo[g]quinoline(?), and 2,4-dimethyl-benzo[f]quinoline (?).

Quantitative analysis of low-temperature tar bases indicated a weight percentage range for individual components of 0.01 (2,3-dimethylpyridine) to 3.41 (2,4,6-trimethylquinoline).

Title: Infrared Spectral-Structural Correlations of Quinolines

Authors: C. Karr, Jr., P. A. Estep and A. J. Papa

Performing Organization: Morgantown Coal Research Center, Morgantown, WV

Sponsoring Agency: Bureau of Mines, U. S. Dept. of Interior, Morgantown, WV

Report No./Journal: J. Am. Chem. Soc., 81, 152 (1959)

NTIS/GPO No.: NA **Type of Report:** Publication

Abstract

This publication describes the relationships for the out of plane hydrogen deformation vibrations in benzenes, naphthalenes, pyridines and quinolines. The purpose of this spectral-structural correlation of quinolines was to aid in the characterization of high boiling, low-temperature bituminous coal tar base distillate fractions consisting of polymethylquinolines. The authors of this article undertook this study with the realization that over 100 isomeric possibilities existed with very few published spectra and no practical possibility of synthesizing all of these compounds. However, only 9 quinolines were synthesized to supplement the few spectral data available from the literature.

Title: Identification of Distillable Tar Acids and Tar Bases from a
Low-Temperature Bituminous Coal Tar

Authors: C. Karr, Jr., P. A. Estep, T. C. L. Chang and J. R. Comberiati

Performing Organization: Morgantown Energy Research Center, Morgantown, WV

Sponsoring Agency: Bureau of Mines, U. S. Dept. of Interior, Morgantown, WV

Report No./Journal: Bulletin 591 (1961)

NTIS/GPO No.: Unknown Type of Report: Government Document

Abstract

This 228 page document contains information on the extensive characterization which was conducted on tar acids and tar bases in a low-temperature bituminous coal tar. Approximately 130 individual compounds were identified mostly with respect to individual isomers and their amounts were determined or estimated in nearly all instances. This report presents detailed descriptions of the separation and qualitative and quantitative procedures for the characterization of the tar acids and bases. These procedures included micro-vacuum fractional distillation, infra-red and ultra-violet spectrofluroimetry, gas-liquid chromatography and countercurrent distribution. Furthermore, descriptions are presented for the synthesis of authentic specimens of tar acids and tar bases. An appendix in this report contains the ultraviolet and infra-red spectra of 189 individual tar acids and tar bases. The predominance of this information was obtained prior to the advent of gas-liquid chromatograph/mass spectrometer combinations.

Title: Bibliography of Tar Bases: Analysis, Production, Synthesis and Utilization

Author: H. W. Wainwright

Performing Organization: Low-Temperature Tar Research Unit, Morgantown Coal Research Center, Morgantown, WV

Sponsoring Agency: Bureau of Mines, U. S. Dept. of Interior, Morgantown, WV

Report No./Journal: Information Circular 8128 (1962)

NTIS/GPO No.: Unknown Type of Report: Government Document

Abstract

This report is a bibliography consisting of literature and patent references from the years 1945-1961 and is divided into the following headings: analysis and composition, production, synthesis and utilization, and separation, purification an properties of constituents in low-temperature coal tar bases. The author indicates that, although over 1,000 references are included, this may not be a comprehensive survey.

Title of Project: Pollutants from Synthetic Fuels Processes

Investigator: Forest Mixon

Specialty: Chemical Engineer

Performing Agency: Research Triangle Institute, Research Triangle
Park, NC 27709

Supporting Agency: Environmental Protection Agency, Industrial
Environmental Research Laboratory, Research
Triangle Park, NC 27711

Agency's Number(s): Unknown

Project Period: 10/1/76 - 9/30/79 Funds: FY76, 77, and 78
Unknown

Summary

The Research Triangle Institute under this program is conducting for the EPA a major research program to study potential pollutants from synthetic fuels operations. The purpose of the research is to develop a fundamental understanding of those factors and conditions which cause the production of environmental pollutants in Synfuels processes and to provide to EPA and to the scientific and technical community the information needed to guide the control of potentially hazardous materials from Synfuels plants of the future.

The research program includes both an experimental and an analytical study. The experimental study includes first the design, fabrication and operation of one or more laboratory reactors to simulate conditions which may be utilized in action Synfuels plants; second, the development and implementation of chemical analysis procedures for the evaluation of elements and compounds that result from Synfuel reactors; third, the screening of the major coals which are available in the U. S.

and characterization of compounds as dependent upon reactor parameters and input coal; and fourth, the determination of the kinetics of formation of the pollutants of significance.

The analytical study provides for utilizing results of the screening tests to project potential human exposure to effluents and emissions from these plants and to establish priority ratings for the various pollutants based upon the extent to which projected exposures are hazardous. The analytical study also provides for an understanding of the reaction kinetics with the view of producing the controls necessary for Synfuels plants.

Title of Project: Environmental Effects from Leaching of Coal Conversion By-Products

Principal Investigator: W. Van Meador and R. Erickson

Specialty: Unknown

Performing Agency: University of Montana; Missoula, MT

Supporting Agency: U. S. Environmental Research and Development Administration

Agency's Number(s): Unknown

Project Period: 6/17/75 - 6/17/78 Funds: FY75 - $74,948

Summary

This program proposes to conduct tests which will characterize the ash and slag materials with regard to the amounts of the more toxic chemical elements that will be released and the rates at which they are released into the environment. Selection of elements to be leached in the hazardous ash dumps have been made from tabulations under the following criteria:

(a) The relative toxicity of the element

(b) The relative concentration of the element in the coal

(c) The likelihood that the element will remain in the ash.

Title of Project: Profiling Trace Elements in Resources and Processes
Involving Water, Coal and Air

Principal Investigator: D. Tolmin, J. Knoeck, J. C. Glass, R. D. Koob,
and D. Doyle

Specialty: Unknown

Performing Agency: Department of Chemistry, North Dakota State
University, Fargo, ND 58102

Supporting Agency: U. S. Department of Interior; Office of Water
Research and Technology

Agency's Number(s): Unknown

Project Period: 7/1/74 - 6/30/75 Funds: FY75 - $31,600

Summary

The proposed research program involved the determining of trace metal composition of the lignite coal mine in the region near southwestern North Dakota and establishing the extent to which such constituents are transferred from the lignite to the water used in the gasification process. The techniques of atomic absorption spectrometry, anodic stripping, voltametry and x-ray fluorescence spectrometry were employed to determine the trace metal composition of: (1) regional water prior to utilization in the gasification process; (2) lignite coal mine in the region; (3) residue remaining after gasification; (4) regional waters after utilization in the gasification process; and (5) stack emissions from gasification plants. The program objectives were to provide a trace metal profile developed for the gasification process and to assess the impact of coal gasification on the trace metal content of water in the West River of North Dakota.

Title of Project: A Survey of Trace Elements in North Dakota Lignite and Effluent Streams from Combustion and Gasification Facilities

Principal Investigator: D. N. Bari

Specialty: Unknown

Performing Agency: Engineering Experimental Station; University of North Dakota; Grand Forks, ND 58201

Supporting Agency: North Dakota State Water Commission, Bismark, ND

Agency's Number(s): Unknown

Project Period: 5/1/74 - 7/31/75 **Funds:** FY74 - Unknown

Summary

One of the concerns of this program is the possible emission into the environment of toxic trace elements originally in the lignite during burning or gasification of lignite in the western part of the state. The trace elements known to be toxic in small amounts are arsenic, beryllium, cadmium, fluorine, lead, mercury and selenium. A survey was to be made of the trace element concentrations in lignites from various North Dakota sources. A survey was made of the work done on the distribution of trace elements in the effluent streams of coal-fired power plants and coal gasification plants. The conclusion according to this program is that for the average amount of mercury present in the lignite, mercury emission in air will be well below the present federal standards.

Title of Project: In Situ Coal Gasification

Principal Investigator: C. F. Bradenburg and G. G. Campbell

Specialty: Unknown

Performing Organization: U. S. ERDA, Laramie Research Center, Laramie, WY, and Sandia Laboratories

Supporting Agency: U. S. Environment Resesearch and Development Administration, Washington, DC

Agency's Number(s): Unknown

Project Period: 7/1/72 - 7/1/82 Funds: FY74 - $686,000

FY75 - $1,576,000

FY76 - $2,800,000

Summary

The first in situ coal gasification experiment in Wyoming was conducted at Hanna from March, 1973 through March, 1974. From September, 1973 through March, 1974, gas production averaged 1.6 mm standard cubic feet per day of 126 but per standard cubic foot of gas. An energy balance for this period indicated four times more energy produced than consumed in operating the experiment.

Title of Project: Characterization of Coal for Open Cycle MHD Power Generation System - Task A

Principal Investigator: F. E. Diebold

Specialty: Engineering

Performing Agency: Montana State College of Mineral Sciences and Technology, Butte, MT

Supporting Agency: U. S. Energy Research and Development Administration Office of Fossil Fuels, Washington, DC

Agency's Number(s): Unknown

Project Period: 4/1/75 - 7/30/76 Funds: FY75 - $118,340

Summary

This program attempted to study and characterize in detail the McKay Simcol to assess its applicability to performance in direct coal fired MHD electrical generation systems. Emphasis was placed on method development for sample analysis coupled with the development of a scheme for geological/chemical mapping. Major inorganic constituents of the coal ash (aluminum, calcium, iron, potassium, magnesium, sodium, silicon and titanium) and trace elements of the coal ash (silver, arsenic, boron, barium, beryllium, cadmium, cobalt, chromium, cesium, copper, gallium, mercury, lanthium, lithanum, manganese, nickel, phosphorus, lead, rubidium, selenium, tin, strontium, uranium, vandium, zinc) were to be analyzed.

Title of Project: Develop Methods to Characterize Heavy Liquids from
Fossil Fuel Energy Sources
Principal Investigator: D. R. Lanthum
Specialty: Unknown
Performing Agency: U. S. ERDA; Laramie Research Center; Laramie, WY
Supporting Agency: U. S. ERDA; Washington, DC
Agency's Number(s): Unknown
Project Period: 7/1/66 - Indefinite

Summary

The objectives of this project are: (1) to develop separation methods to prepare analytically significant fractions from petroleum residues, tar sand bitumens and liquids from coal and oil shale; (2) to develop techniques to characterize the major compound types in each fraction; (3) to develop information on compound type relationships among the fossil fuel energy sources; and (4) to apply this information in solving the problems of efficient utilization of these materials as an energy source. A separation/characterization method that was developed for high boiling petroleum distillates will be tested under this program and modified and applied to the materials listed above. The characterization data obtained are needed in efficiently utilizing the materials in environmental and exploration studies.

Title of Project: Waste Water Effluents for the Synthane Coal Gasification Process

Principal Investigator: R. W. Dunlap and M. J. Massey

Performing Organization: Carnegie-Mellon University, Institute of
Technology, Frew Avenue and Margaret Morrison,
Pittsburgh, PA 15213

Supporting Agency: U. S. Department of Intrior, Bureau of Mines

Agency's Number(s): Unknown

Project Period: 7/74 - 2/75 **Funds:** FY75 - Unknown

Summary

This program utilized the Bureau pilot plant (Synthane oxygen steam coal gasifier) and determined the effects of coal reaction temperature and residence time on the quantity of tar and aqueous effluent produced during gasification. Three types of injection geometry of the coal into the gasifier were studied. In each series of experiments, the quantities of tar and aqueous condensates leaving the gasifier were measured. The compositions of each of these condensates was determined, *e.g.*, ammonia, phenol, COD, POD, ACN, etc. The specific component identification of organics and elemental substances under this project is not indicated.

Title of Project: Characterization of Ash from Various Coal Gasification Processes

Principal Investigator: R. D. Harvey and J. Yeruskhalmi

Specialty: Unknown

Performing Agency: State Geological Survey, National Resources Bldg.,
Urbana, IL 61801

Supporting Agency: City University of New York

Agency's Number(s): Unknown

Project Period: 7/74 - 6/75 **Funds:** FY75 - Unknown
Multi-support

Summary

The proposed program will investigate structural mineralogy and chemical characteristics of coal and agglomerates of ash and clinkers produced in various stages of operation of three foreign Ignifluid boilers. The aim of the study is to determine if the coals used and the ash material produced will have unique properties that should dictate caution in the operation of an Ignifluid boiler using Illinois coals. The mechanism of the formation of the ash agglomerates and the distribution of the composition of the glassy matrix and of the various types of enclosed fragments are proposed for study. The analytical techniques to be used are: polarized light microscopy and electron microscopy with x-ray spectrographic analyses.

Title of Project: Environmental Aspects of Slagging Fixed Bed Coal High BTU Gasification Process

Principal Investigator: R. C. Helman, M. M. Fegley and S. A. Codey

Performing Agency: U. S. Energy Research and Development Administration
Grand Forks Energy Research Center, Grand Forks, ND
58201

Agency's Number(s): Unknown

Project Period: 1/1/74 - indefinite **Funds:** FY75 - $230,000

Summary

The objectives of this program are to determine the type, amount and pollution aspects of liquid, gaseous and particulate effluents produced in the high BTU gasification of western coals in a slagging fixed bed gasifier. The organic constituents in these effluents are proposed to be analyzed by gas chromatography/mass spectrometry.

Title of Project: Slagging Fixed Bed Coal Gasification

Principal Investigator: R. C. Ellman

Performing Agency: U. S. ERDA, Grand Forks Energy Research Center,
Grand Forks, ND 58202

Supporting Agency: U. S. ERDA

Agency's Number(s): Unknown

Project Period: 7/1/74 - 6/30/80 Funds: FY75 - $180,000
FY76 - $600,000

Summary

The objectives of this program are to operate a fixed bed slagging coal gasification unit to study the effluents during operation with lignite and other low rank coals; to develop methods to reduce adverse environmental effects from water usage; to determine gasification characterics of selected western coals and to develop techniques to reduce or remove limitations of particle feed size and moisture content in fixed bed gasification systems.

Title of Project: Coal Hydrogenation and Hydrocracking Using a Metal Chloride Gaseous AGL Catalyst System

Principal Investigator: F. P. McCandless

Specialty: Engineering

Performing Agency: Montana State University, Department of Chemical Engineering, Bozeman, MT 59715

Supporting Agency: National Science Foundation, Washington, DC

Project Period: 7/1/75 - 6/30/77 Funds: $55,959

Summary

This program is primarily concerned with the examination of the optimum criteria for the hydrogenation and hydrocracking of coal. One of the objectives of this program includes the complete characterization of liquid, gas and unreacted coal products during the energy conversion process. The analytical tools to be employed for analysis of these by-products are not indicated nor does it indicate whether elemental or organic compounds will be examined.

Title: Characterization of Effluents from Coal Fired Utility Boilers

Authors: B. G. McKinney and H. B. Flora

Performing Organization: Tennessee Valley Authority, Power Research Staff, Chattanooga, TN 37401

Sponsoring Agency: Control Systems Laboratory, Environmental Protection Agency, Research Triangle Park, NC 27711

Report No./Journal: Quarterly Progress Report Nos. 1-5 for the periods July 25, 1975 to July 25, 1976

NTIS/GPO No.: None　　Type of Report: Quarterly

Abstract

The objectives of this project are to: (1) characterize coal pile drainage; (2) assess the effect of pH adjustment on ash pond effluent; (3) assess and then design an effective program for monitoring ash pond effluent; (4) evaluate chlorinated water effluent quality from an once thorough cooling system; (5) assess, characterize and quantify coal ash leachate effects on ground water quality; and (6) study gaseous and particulate emissions from several types of boilers. The project scope included: (1) characterization and quantification of the chemical and physical components of coal pile drainage; (2) assessment and quantification of the chemical and physical composition of ash pond effluent after the pH of the ash pond had been adjusted; (3) evaluation of an ash monitoring program to determine the sample necessary to obtain reliable qualitative and quantitative information; (4) assessment, characterization and quantification of coal ash leachage effects on ground water; (5) quantification and evaluation of chlorinated effluent from once through cooling systems; and (6) characterization of gaseous and particulate effluents from tangential wall fired and cyclone units.

This program has presented in these reports the characterization of many elemental compounds for the various circumstances described above.

Title: Trace Elements in a Combustion System

Authors: R. W. Coutant, J. S. McNulty and R. D. Giammar

Performing Organization: Battelle Columbus, 505 King Avenue, Columbus, OH 43201

Sponsoring Agency: Electric Power Research Institute, 3412 Hillview Avenue, Palo Alto, CA 94303

Report No./Journal: EPRI-122-1

NTIS/GPO No.: None Type of Report: Final, January, 1975

Abstract

The objective of this program was to determine the distribution of 12 trace elements: As, Be, Cd, Cr, Cu, Hg, Mn, Ni, Pb, Se, V and Zn among the products of combustion from four types of coal which were burned in the Battelle multifuel furnace facility which simulates the time-temperature profiles typical of a conventional station. This report states that the more volatile trace elements As, Hg, Pb and Se tended to concentrate in the products that would be emitted normally from the stack. The less volatile elements were distributed more or less uniformly in the slag, ash deposit and precipitator catches. This study addressed only elemental analysis; the characterization of the organic constituents in these by-products was not performed. The instrumental techniques used for determining the elements were not discussed.

Title: Characterization and Utilization of Municipal and Utility
Sludges and Ashes. Vol. III: Utility Coal Ash
Authors: N. L. Hecht and D. S. Duvall
Performing Organization: University of Dayton Research Institute,
300 College Park Dr., Dayton, OH 45469
Sponsoring Agency: National Environmental Research Center, Office
of Research and Development, U. S. Environmental
Protection Agency, Cincinnati, OH 45268
Report No./Journal: EPA-670/2-75-033C
NTIS/GPO No.: PB-244-312 Type of Report: Final Government Technical

Abstract

This research program defined the nature of the coal ash, i.e., the quantities produced and the locations of the major utilities generating the coal ash. Data are presented on the inorganic composition of ash consisting primarily of the following inorganic compounds: silicon dioxide, aluminum oxide, ferric oxide, titanium dioxide, phosphorus pentoxide, calcium oxide, magnesium oxide, sodium oxide, potassium oxide and sulfite. Data on these inorganic compounds are listed for electric utilities utilizing coal in the New England mid-Atlantic, east North Central, west North Central, South Atlantic, east South Central, west South Central, mountain and Pacific States. Also included are the major chemical constituents of coal ash which are primarily the elemental compounds, silica, aluminum, iron, calcium, magnesium, titanium, potassium, sodium, boron, phosphorus, manganese, molybdenum, zinc, copper, mercury, uranium, and thorium.

Title: Characterization and Utilization of Municipal and Utility
Sludges and Ashes. Vol. I: Summary

Authors: N. L. Hecht and D. S. Duvall

Performing Organization: University of Dayton Research Institute,
300 College Park Ave., Dayton, OH 45469

Sponsoring Agency: National Environmental Research Center, Office
of Research and Development, U. S. Environmental
Protection Agency, Cincinnati, OH 45268

Report No./Journal: EPA-670/2-75-033A

NTIS/GPO No.: PB-244-310 Type of Report: Final Government Technical

Abstract

Burning of coal produces an ash residue which is derived from the inorganic material constituents in the coal and the organic material not completely burned. In coal burning utility boilers, the coal ash residue is collected from the bottom of the boiler unit (bottom ash) and from the air pollution equipment through which the stack gases pass (fly ash). The largest concentration of power plants is in the mid-Atlantic and the east north central states. There are a very few coal burning power plants west of the Mississippi River.

The coal ash residues recovered from the boiler units are primarily iron, aluminum, and silicates with additional amounts of lime and magnesium, sulfur trioxide, sodium oxide, potassium oxide and carbon. This summary presents an average chemical analysis for coal ash.

Title: Southwest Energy Study Coal Research Work Group. Part I: Coal Resources and Reserves of the Southwestern United States. Part II: Composition and Trace Element Content of Coal and Power Plant Ash

Authors: P. Averitt, A. V. Bailey, G. H. Horn, A. A. Mattila, J. W. Moffitt, A. B. Nichelson, W. C. Sheldon, M. T. Smith and J. B. Storrs

Performing Organization: U. S. Geological Survey

Sponsoring Agency: U. S. Dept. of Interior

Report No./Journal: Appendix J, January, 1972

NTIS/GPO No.: Unknown Type of Report: Technical Government Report on the Coal Resources Work Group

Abstract

The specific objective of this study was to examine the elemental and inorganic composition of coal that is burned or to be burned at the ten major electricity generating plants and fly ash and bottom ash. The five power plants that were studied were: Four Corners, NM, Cholla, AZ, Mohave, NV, Hayden, CO and Naughton, WY. Also five power plants which are planned or under construction are listed. These are: San Juan, NM, Navajo, AZ, Kaiparowits, UT, Huntington Canyon, UT and Jim Bridger, WY. The source and geological designation of seventy-one coal samples that were chemically analyzed were presented.

The methods used for elemental analysis were: wet chemical, x-ray fluorescence, spectrographic, atomic absorption, selected ion electrode and neutron activation techniques. A comparison between these techniques in the analysis of the various coals and fly ash material is also included.

Sixteen samples of fly ash and furnace bottom ash from the five power plants were analyzed for 46 elements. The conclusion from these data is that the analysis reveals that large amounts of the critical elements are trapped in the fly ash by the scrubbers and precipitators in the stack. Only relatively small amounts of these elements accumulate in the bottom ash. The elements markedly concentrated in fly ash relative to bottom ash were antimony, arsenic, fluorine, mercury, selenium, tellurium and thallium. Copper, chromium, molybdenum, nickel, lead and vanadium as well as boron, gallium, scandium and to a slight degree sulfur were also found concentrated in fly ash relative to bottom ash.

No attempt was made to analyze for or to evaluate the possible formation of hydrocarbons, mercaptans or similar organic components that might not be combusted and therefore escape into the final effluents. A schematic was presented on the cycle of materials into and the products out of the power plant. The materials into the power plant were oxygen, coal and water. The materials out were ash, gaseous material and volatiles, processed water, heat and electricity. The ash can be divided into fly ash and bottom ash, which normally is dumped into strip pits. Associated with the strip pits is natural water drainage. Some of the processed water may be recycled as water input into the power plant with a portion lost as steam through evaporation or as an ash slurry or through seepage.

Title: The Impact of Coal-Fired Power Plants on the Environment

Authors: James L. Clapp, Daniel E. Willard and Richard J. Timm

Performing Organization: Environmental Monitoring and Data Acquisition Group, Institute for Environmental Studies, University of Wisconsin, Madison and State of Wisconsin Public Service Commission Medical College of Wisconsin

Sponsoring Agency: U. S. Environmental Protection Agency

Report No./Journal: EPA Grant R803971010

NTIS/GPO No.: Unknown Type of Report: Technical Quarterly Progress Report, July 21-November 1, 1975

Abstract

The study site is a 527,000 kilowatt coal-fired electric generating station at the Columbis Plant site located four miles south of the city of Portage, WI in the west central portion of Columbia county. The plant is a joint venture between Wisconsin Power and Light Co., Madison Gas and Electric Co. and the Wisconsin Public Service Corp.

The report discusses aquatic chemistry, trace chemical analysis, aquatic invertebrates and fish, ecology for plants and vertebrates, hydrogeology, air pollution modeling, plant vegetation damage, meteorology, land use, visional changes and esthetics and hazardous chemicals in fish.

In this report the analysis of fly ash was presented from each of three stages of the precipitator which was used at the power plant site. It was the purpose of these analyses to characterize the fly ash being discharged into the ash pond. The fly ash from the first stage

precipitator was being sold for commercial use, while the material from the last two stages was slurried with the water and pumped into the ash pond. A total of 32 elements was quantitated in the first, second and third stages of the precipitator. The concentration of trace elements in the samples of suspended particulate matter collected from the ash pond and its drainage system was also determined. A total of 28 elements was analyzed. All of the analyses reported used instrumental and radiochemical neutron activation.

Title: Contribution of Major and Minor Elements to Soils and Vegetation by the Coal-Fired Four Corners Power Plant, San Juan County, NM

Authors: H. L. Cannon and V. E. Swanson

Performing Organization: U. S. Geological Survey, Denver, CO 80225

Sponsoring Agency: U. S. Dept. of Interior, Washington, DC

Report No./Journal: 75-170

NTIS/GPO No.: Unknown Type of Report: Draft Report, 1973

Abstract

The major components in the ash from the four corners coal-fired power plant in San Juan County, NM were found to be potassium oxide, calcium oxide, magnesium oxide, aluminum oxide, silicon dioxide, sodium oxide and iron oxide. Many minor elements were also determined including antimony, arsenic, fluorine, mercury, selenium, tellurium, uranium and zinc, which was found to be enriched in the fly ash relative to bottom ash or coal.

The analytical methods which were used in this program for the determination of elements were: emission spectroscopy, spectrophotometry, atomic absorption, specific ion electrodes, elemental analyzer, flame photometer, combustion iodometric titration, x-ray spectroscopy, catalysis and neutron activation.

Title: Pathways of Thirty-Seven Trace Elements Through Coal-Fired
Power Plant

Authors: D. H. Klein, A. W. Andren, J. A. Carter, J. F. Emery,
C. Feldman, W. Fulkerson, W. S. Lyon, G. C. Ogle,
Y. Talmi, R. I. Van Hook and N. Bolton

Performing Organization: Oak Ridge National Laboratory, Oak Ridge,
Tennessee 37830

Sponsoring Agency: Unknown

Report No./Journal: Environmental Science and Technology, 9, 973
(1975)

NTIS/GPO No.: None Type of Report: Literature Publication

Abstract

This paper describes the analysis of a suite of elements in coal, fly ash, slag and combustion gases from a large cyclone-fed power plant. Mass balance data for the 37 elements were obtained on the T.A. Allen Steam Plant in Memphis, TN, a part of the Tennessee Valley Authority Electrical Generating System. Mercury, selenium and chlorine and bromine were discharged to the atmosphere as gases. Arsenic, cadmium, copper, gallium, molybdenum, lead, antimony, selenium and zinc were concentrated in fly ash compared to the slag and were more concentrated in the ash discharged through the stack than in that collected by the precipitator. Aluminum, Ba, Ca, Ce, Co, Eu, Fe, Hf, K, La, Mg, Mn, Rb, Sc, Si, Sn, Sr, Ta, and Ti showed little preferential partitioning between the slag and the collected discharge fly ash.

No analysis for organic components was presented. The analytical techniques employed were: neutron activation analysis for most of the elements and isotope dilution spark-source mass spectrometry for Cd, Pb and Zn and flameless atomic absorption for Hg. The Se analyses were done by a newly developed method, gas chromatography with microwave emission spectrometric detector. Copper, Ga, Ni and Sr were determined by a new absolute high sensitivity x-ray fluorescence technique using monochromatic x-rays for excitation.

Title: Coal-Fired Power Plant Trace Element Study: A Three Station
Comparison
Authors: F. G. Mesich and K. Schwitzgebel
Performing Organization: Radium Corporation, Austin, TX
Sponsoring Agency: U. S. Environmental Protection Agency, Region VIII
Denver, CO
Report No./Journal: Vol. I (TS-1a)
NTIS/GPO No.: Unknown Type of Report: Annual, September, 1975

Abstract

This report summarizes the results of the determination of trace elements in coal ash, fly ash and vapors in the flue gas of three coal-fired electric generating stations.

A material balance approach was used for quantitating 27 elements in the coal-fired generating station and 26 additional elements were determined semi-quantitatively. Samples which were analyzed quantitatively (27 trace and minor elements) were determined by the following techniques: (a) atomic absorption spectroscopy; (b) x-ray fluorescence; (c) ion selective electrodes; (d) fluorimetry; and (e) colorimetry. The sample types which were examined at the three plants were: coal, coal ash and sludge, lime, and aqueous effluent including a WEP liquor. Semi-quantitative analyses for 53 elements were obtained by spark-source mass spectrometry.

Station 1 plant consisted of four individual units with a generating capacity of 750 MW fired with Wyoming sub-bituminous coal. Unit No. 4 was sampled for this program. Station 2 contained a 350 MW boiler tangentially fired with Wyoming sub-bituminous coal. Station 3 was

fired with a North Dakota lignite in a 250 MW cyclonic boiler with mechanical cyclone particulate collectors.

Title: Coal-Fired Power Plant Trace Element Study: Station 1, 2
and 3

Authors: F. G. Mesich and K. Schwitzgebel

Performing Organization: Radium Corporation, Austin, TX

Sponsoring Agency: U. S. Environmental Protection Agency, Rocky
Mountain Prairie Region, Region VIII, Denver, CO

Report No./Journal: Vol. II (Ts-1b)

NTIS/GPO No.: Unknown Type of Report: Annual, September, 1975

Abstract

This volume is one of four volumes comprising the document described as coal-fired power plant trace element study prepared for EPA under Contract 68-01-2663. A description of the overall program was provided in the previous abstract.

Title: Trace Element Study in a Pulverized-Coal-Fired Power Plant

Authors: J. Kaakinen

Performing Organization: Department of Chemical Engineering, Univ.
of Colorado, Boulder, CO

Sponsoring Agency: National Science Foundation (RANN), Washington, DC

Report No./Journal: University Microfilms Ann Arbor, MI 48106
University Microfilms No. 75-3795

NTIS/GPO No.: Unknown Type of Report: Thesis, Ph.D.

Abstract

A study of 18 elements in the inlet coal and the outlet water in ash streams including flow gas particulates of a coal-fired power plant was performed. Mass balance data were obtained within ±10% for 9 elements; aluminum, iron, copper, zinc, rubidium, strontium, yttrium, zirconium, and niobium, as well as for four trace substances; mercury, plutonium, lead and radium. Samples were obtained from Unit No. 5 of the Valmont Power Station located near Boulder, CO which is owned by the Public Service Co. of Colorado.

The analytical techniques used for determining the elemental composition of effluents from the coal fired power plants were: (1) colorimetric wet chemistry (molybdenum); (2) atomic absorption spectrophotometry (iron and aluminum); (3) x-ray fluorescence spectroscopy (iron, copper, zinc, gallium, arsenic, selenium, rubidium, strontium, yttrium, zirconium, molybdenum, tin, lead, Nb, Sb and other elements) and (4) radioisotopic determination (^{210}Pb, ^{210}Mo and ^{226}Ra).

This study presents chapters which idscuss the following: (1) power plant site and sample collection; (2) sample preparation and analysis results; (3) mercury: measurements, results and discussion;

(4) mass balances of trace elements; (5) trace element distribution patterns; (2) mechanism for observed volatilization and enrichment of elements; and (7) trace element removal performance of the control devices used.

Title: Spark Source Mass Spectrometer Investigation of Coal Particles
and Coal Ash
Authors: T. Kessler, A. G. Sharkey, Jr. and R. A. Friedel
Performing Organization: Pittsburgh Energy Research Center, Pitts
bugh, PA
Sponsoring Agency: U. S. Department of Interior
Report No./Journal: TPR-42
NTIS/GPO No.: Unknown Type of Report: Government Technical
Progress Report

Abstract

Spark source mass spectrometry was used to determine the amounts of minor and trace elements in coal particles of various sizes including those in the respirable range (< 5 microns). Fifty-six elements ranging in concentration from 0.1 ppm wt. - 5,000 ppm wt. were determined. The investigation of coal and coal ash showed that the organic material in coal does not interfere with the spark source determination of the various elements.

Title: Fate of Some Trace Elements During Coal Pretreatment and
Combustion

Authors: A. Schultz, E. A. Hattman and W. B. Booher

Performing Organization: Dept. of Interior, Pittsburgh, PA 15213

Sponsoring Agency: ERDA

Report No./Journal: Trace Elements in Fuel, pg. 139-153, Publisher:
American Chemical Society, Washington, DC, 1975

NTIS/GPO No.: None Type of Report: Adv. in Chemistry Series 141

Abstract

This program presents results on studies which have shown that it is possible to remove many of the potentially toxic trace elements present in coal when the mineral matter is produced by coal washing. As part of the program, analytical chemical techniques have been developed to determine Hg, Cu, Cr, Mg, Ni, Cd, Pb and F in coal and fly ash.

Title: New Knowledge Concerning the Properties of Fly Dust from Coking Plants, No. 4. Bituminous Coal Tar Distillation Plants

Authors: V. Masek

Performing Organization: Unknown

Sponsoring Agency: Unknown

Report No./Journal: Zentralbl. Arbeitsmed. Arbeitsschutz, Vol. 22, 11, pg. 323-337, 1972

NTIS/GPO No.: None **Type of Report:** Literature Publication

Abstract

At twenty locations of three Czechoslovakian coal tar distillation plants, the concentration of dust and of 3,4-benzpyrene in the fly dust were determined.

Title of Project: Study of Disposal of By-Products from Throw Away Desulfurization Systems

Principal Investigator: J. Meltzer and J. Rossoff

Specialty: Unknown

Performing Agency: Aerospace Corporation, P. O. Box 95085, Los Angeles, CA 90045

Supporting Agency: U. S. Environmental Protection Agency, Control Systems Lab Division, Research Triangle Park, NC 27711

Agency's Number(s): Unknown

Project Period: 7/75 - 11/76 Funds: FY76 - Unknown

Summary

In this study the Aerospace Corporation is conducting laboratory experimentation and engineering surveys and analyses regarding the disposal of desulfurization sludges from coal burning power plants. The physical characterization of the sludges to evaluate the potentially toxic hazards posed in processing or procedures that may be performed in subsequent handling, disposal or utilization of the sludge. The sludges to be examined will be obtained from plants burning eastern and western coal and using limestone, lime and a double alkaline absorbent material for the desulfurization process.

Title of Project: Methods of Analysis of Liquid Effluent from Carbonization Plants

Principal Investigator: R. L. Cooper and J. D. Norris

Specialty: Environmental Studies Section

Performing Agency: British Carbonization Research, Chesterfield
England, United Kingdom

Supporting Agency: United Kingdom

Agency's Number(s): Unknown

Project Period: 7/74 - 6/75 **Funds:** FY75 - Unknown

Summary

This program is concerned with the development and assessment of accuracies and precisions of reference and routine methods for determining organi and inorganic constituents. This will include COD, TOC, phenols, etc., but not specific organics. The routine methods to be studied will not include the specific constituent characterization (organic and inorganic) in the samples.

Title of Project: The Characterization of Hazardous Materials Emitted from Coal Combustion and Conversion

Principal Investigator: G. E. Rolfe and D. F. Natusch

Specialty: Chemistry

Performing Agency: University of Illinois, School of Chemical Sciences
Urbana, IL 61801

Supporting Agency: U. S. National Science Foundation, Division of Advanced Energy Research and Technology

Agency's Number(s): ERT-74276

Project Period: 10/75 - 12/76 Funds: FY76 - Unknown (Previous Funding for FY73, FY74, FY75 was $125,000)

Summary

The proposed research is directed towards the characterization of toxic materials emitted in effluents from coal conversion and combustion operations. The specific aim is to elucidate the basic principles which govern formation and release of toxic trace metals in carcinogenic organic species during power generation. The analytical methodology to be employed in this program was not delineated.

Studies currently under progress are directed towards establishing the mechanisms whereby toxic species become associated with particulate matter and towards establishing an environmental impact of these materials. On this basis it is concluded that most of the organic analysis will be associated with air pollution, specifically particulate matter.

Title of Project: Trace Element Effects of Energy Conversion Facilities

Principal Investigator: G. A. Christensen

Performing Agency: North Dakota State Department of Health, Division
of Environmental Engineering, Bismark, ND 58505

Supporting Agency: Old West Regional Commission, Frat Bldg., Suite 306A
Billings, Montana 59101

Agency's Number(s): 10570168

Project Period: 6/25/75 - 6/30/77 Funds: FY76 - $55,000
FY77 - $45,000

Summary

The purpose of this project is to examine the food chain aspects of trace elements emitted from energy conversion facilities. Among the many specific aims, one of the purposes of this program is to determine the chemical profile of trace elements in soil reservoir from existing coal-fired power plants. The extent of element analysis is not provided.

Title: Water Pollution Potential of Mine Spoils in the Rocky Mountain Region

Authors: D. B. McWhorter, R. K. Skogerboe and G. B. Skogerboe

Performing Organization: Departments of Agricultural Engineering and
Chemistry; Colorado State University
Fort Collins, CO

Sponsoring Agency: U. S. Environmental Protection Agency, Grant No. R802621

Report No./Journal: Paper presented at 5th Symposium on Coal Mine Drainage Research

NTIS/GPO No.: None **Type of Report:** Publication

Abstract

Water quality data on runoff, percolate, and leachate are presented. The main emphasis is placed on elemental analysis.

Title: Coal and Coal Mine Drainage

Authors: J. F. Boyer and V. E. Gleason

Performing Organization: Bituminous Coal Research Incorporated
Monroeville, PA

Sponsoring Agency: Unknown

Report No./Journal: Journal Water Pollution Control Federation,
Volume 47, No. 6, June, 1975

NTIS/GPO No.: None

Abstract

This report presents a literature review on coal and coal mine drainage. These reviewed articles cover: (1) formation; (2) effects; (3) abatement; and (4) treatment. The majority of the types of analyses performed on mine drainage center on the elemental analysis of runoff and leachates.

Title of Project: Evaluation of Ground Water Pollution from Eastern Underground Coal Mine

Principal Investigator: Unknown

Specialty: Unknown

Performing Agency: Geraghty and Miller Incorporated, Port Washington, NY 11050

Supporting Agency: United States Environmental Protection Agency, Cincinnati, OH

Contract No.: 68-03-2467

Project Period: Unknown **Funds:** FY76 - $203,800

Summary

A summary is not available on this program.

Title: Detection of Organic Compounds in Respirable Dust

Authors: J. L. Schultz, R. A. Friedel and A. G. Sharkey, Jr.

Performing Organization: Pittsburgh Energy Research Center, Pittsburgh, PA

Sponsoring Agency: U. S. Energy Research and Development Administration, Pittsburgh, PA

Report No./Journal: PERC/RI-75/4

NTIS/GPO No.: Unknown Type of Report: Government Technical Progress Report

Abstract

This report describes the use of high resolution mass spectrometry to analyze the organic material in respiratory size coal dust and mine dust. The objective of this project was to identify and classify the organic compounds in respirable mine dust obtained from mining regions of high and low incidences of coal workers pneumoconiosis. Mass spectral data were obtained for 21 respirable mine dust and 6 respirable size coal dust samples. The predominant organic material consisted of aliphatic, perhydroaromatic, hydroaromatic and aromatic compounds as well as oxygen and olefinic organics.

Title: Detection of Organic Compounds in Respiratory Coal Dust by High
Resolution Mass Spectrometry

Authors: J. L. Schultz, R. A. Friedel and A. G. Sharkey, Jr.

Performing Organization: Pittsburgh Energy Research Center, Pitts
burgh, PA

Sponsoring Agency: U. S. Department of Interior

Report No./Journal: TRP 61

NTIS/GPO No.: Unknown Type of Report: Government Technical
Progress Report

Abstract

An investigation of organic compounds in respiratory coal dust by high resolution mass spectrometry in this report showed organic components which differ by the particle size, rank of coal, coal of the same rank from different coal seams and irrespirable mine dust and respirable coal dust from the same mine. The 8 respirable mine dust samples that were studied were from the coal seams in the Appalachian region. The molecular weights of the major organic compounds varied greatly among these respirable mine dusts. Three of these mine dusts contained a high concentration of polynuclear aromatic hydrocarbons.

Title: A Survey of the Most Recent Applications of Spark-Source
Mass Spectrometry

Authors: R. Brown, M. L. Jacobs and R. E. Taylor

Performing Organization: Analytical Service, Acculabs Inc., Denver, CO

Sponsoring Agency: Health Services and Mental Health Administration,
Dept. of Health, Cincinnati, OH

Report No./Journal: None

NTIS/GPO No.: None Type of Report: In-House

Abstract

Although this publication discusses principally the application of spark-source mass spectrometry to the analysis of several different matrices, e.g., coal, coal dust, lung tissue, particulate matter from mining interiors and particulate matter from welding shops, it does also present the typical trace elements found in fly ash. A total of 65 elements in fly ash from a coal-fired power plant was analyzed by this technique.

Title: Trace Elements in Coal Dust by Spark-Source Mass Spectrometry

Authors: A. G. Sharkey, Jr., T. Kessler and R. A. Friedel

Performing Organization: Spectrophysics, Pittsburgh Energy Research Center, 4800 Forbes Ave., Pittsburgh, PA 15213

Sponsoring Agency: Energy Research and Development Administration, Washington, DC

Report No./Journal: Advances in Chemistry Series, No. 141, 48-56 (1975)

NTIS/GPO No.: Unknown Type of Report: Chapter in Trace Elements in Fuel, ACS, Adv. Chem. Ser. 141 (1975)

Abstract

This research article discusses a method for determining trace elements in 10 pairs in respirable range mine dust and prepared coal dust using the technique of spark-source mass spectrometry. Samples representing eight coal seams in Pennsylvania, West Virginia, Virginia and Utah were analyzed. For a majority of the sample pairs, several elements including silver, cadmium, copper, chromium, calcium, chlorine, phosphorus and bromine show higher values in the mine dust than the coal. A limited investigation was conducted on the organic material associated with the mine dust which indicates an additional series of highly saturated materials not derived from coal.

Title: Occurrence and Distribution of Potentially Volatile Trace
Elements in Coal

Authors: R. R. Ruch, A. J. Gluskoter and N. F. Shimp

Performing Organization: Illinois State Geological Survey

Sponsoring Agency: U. S. Environmental Protection Agency, Clean Fuels
and Energy Branch, Control Systems Lab., Research
Triangle Park, NC

Report No./Journal: August, 1974

NTIS/GPO No.: Unknown Type of Report: Final Government
Technical

Abstract

The results on the development of accurate and reliable data on elemental analysis of coal and coal ash are discussed. Of particular interest is the presentation of a comparison of a series of techniques for the determination of elements in fly ash. The methods of analyses employed and compared were: x-ray fluorescence, optical emission spectrophotometry, atomic absorption spectrophotometry, neutron activation and ion selective electrodes. The trace elements analyzed were: antimony, arsenic, beryllium, boron, bromine, cadmium, chromium, cobalt, copper, fluorine, gallium, germanium, lead, manganese, molybdenum, nickel, mercury, phosphosus, selenium, tin, vanadium, zinc and zirconium. Major and minor elements also analyzed were: aluminum, calcium, chlorine, iron, magnesium, potassium, silicon, sodium, sulfur and titanium.

Title of Project: Laboratory Leaching Studies of Coal Mine Spoil Material

Principal Investigator: G. K. Pagenkopf

Performing Agency: Montana State University, Department of Chemistry, Bozeman, MT

Supporting Agency: U. S. Environmental Protection Agency, Region VIII
Denver, CO 80201

Project Period: 3/1/74 - 6/30/74 Funds: $2,495

Summary

The objective of this study was to provide quantitative chemical and physical data regarding the leachability of coal spoil materials and how that leachability may affect the quality of shallow ground water supplied in the northern great plains. The study would primarily concentrate on soluble inorganic salts in these leachates. A description of the analytical methodology to be employed was not given.

Title of Project: Column Leaching Studies of Coal Mine Spoil Material

Principal Investigator: Gordon K. Pagenkopf

Specialty: Associate Professor

Performing Organization: Montana State University, Department of Chemistry, Bozeman, Montana 79515

Supporting Agency: U. S. Environmental Protection Agency, Office of Energy Activity, 1860 Lincoln, Denver, CO 80203

Agency's Number(s): DEA-75-27B

Project Period: 2/1/75 - 6/30/76 Funds: $2,495

Summary

The proposed work is to examine the possibilities of coal mine spoil material yielding salt to the ground water. No details are available with regard to the specific types of inorganic materials to be studied.

Title of Project: Hydrologic Characteristics of Mine Spoils

Principal Investigator: W. A. Van Voast

Specialty: Hydrologist

Performing Organization: Montana Bureau of Mines and Geology

Supporting Agency: Old West Regional Commission, Frat Bldg., Suite
306A, Billings, Montana 59101

Agency's Number(s): 10570165

Project Period: 6/16/75 - 6/30/77 Funds: $97,400

Summary

One of the objectives of this program is to collect water samples from research wells, ponds and seeps where a concentration of major chemical constituents including trace metals and dissolved organic compounds may be occurring which is associated with mine spoils. A part of this program will involve the assimilation and laboratory leach test to predict future spoils, *i.e.*, water quality. The water chemistry research is proposed to include: (1) analysis of mine waters for organic compounds dissolved from coal and their roles in chelation and mobilization of trace metals in mine waters; (2) the major chemical analyses for calcium, magnesium, sodium, sulfate, bicarbonate and chlorides as well as trace metal analysis for lead, zinc, chromium, copper and selenium.

Title of Project: A Study of Coal Associated Waste Resulting from the
Mining, Processing and Utilization of Coal
Principal Investigator: J. W. Leonard, K. K. Humphreys, R. B. Muter,
J. F. Slonaker, W. F. Lawrence, and W. Buttermore
Specialty: Coal Research
Performing Agency: West Virginia University, School of Mines, Morgantown, WV 26506
Supporting Agency: U. S. Dept. of Interior, Office of Coal Research
Agency's Number(s): Contract 14-32-001-1218
Project Period: 7/74 - 6/75 Funds: FY75 - Unknown

Summary

The research at West Virginia University has been concerned with investigating all waste and by-products associated with the conversion and utilization of coal. The proposed objectives of the programs are: (1) to characterize coal associated waste both chemically and physically; (2) to propose and investigate possible utilization processes; (3) to suggest safe disposal methods for these materials; and (4) to describe their environmental impact.

The coal-associated wastes under study include coal preparation waste, such as gob in coal fines; acid mine drainage; treatment waste; modified fly ash and other lime/limestone waste resulting from sulfur dioxide abatement processes; coal ashes and those wastes which may result from the various conversion processes.

Title of Project: Environmental Effects from Leaching of Coal Conversion By-Products

Principal Investigator: W. P. VanMeter and R. E. Erickson

Specialty: Chemistry

Performing Agency: University of Montana, School of Arts and Sciences
770 Eddie Street, Missoula, MT 59801

Supporting Agency: U. S. Energy and Development Administration,
Advanced Research and Support Technology Division

Agency's Number(s): Contract E-49-(18)-2019

Project Period: 6/75 - 6/76 Funds: FY75 - $8,327

Summary

This project proposes to examine solid waste materials obtained from existing pilot plants which are under operation for gasification of coal. It is the purpose of this program to determine the characteristics of the material which may leach through the action of precipitation or ground water. The elements to be determined will include barium, cadmium, mercury, nickel, lead, selenium, manganese, strontium and fluorine.

Title of Project: Geochemical Survey of Waters of the Western Coal Regions

Principal Investigator: G. L. Feder

Specialty: Water Resources Division

Performing Agency: U. S. Dept. of Interior, Geology Survey, Denver, Co 80225

Supporting Agency: U. S. Dept. of Interior, Geological Survey, Waters Resources Division

Agency's Number(s): CROO-095

Project Period: 7/74 - 6/75 Funds: FY75 - $47,000

Summary

The projected goal of this program is to obtain data on the natural and pre-development biochemistry of the waters of the area with particular emphasis on trace elements that might have a relationship to health and disease in humans or animals. The objective is to quantify changes already produced by existing developments in the area between soil plants, rocks and waters which are associated with strip mining and power production.

Title of Project: State of the Art Evaluation of Petroleum and Coal Waste

Principal Investigator: L. Streebin

Specialty: Engineering

Performing Agency: University of Oklahoma, Research Institute,
202 West Boyd, Rm. 101, Norman, Oklahoma 73069

Supporting Agency: U. S. Environmental Protection Agency, Office of Research and Development

Agency's Number(s): 12050-DKF & 72PT0807

Project Period: 7/74 - 6/75 **Funds:** FY75 Unknown

Summary

The final report of this study presents a state of the art evaluation of pollution problems, abatement procedures, and control techniques relevant to the petroleum and coal industries. The principal pollutants in water discharge from the processing of coal were determined to be suspended solids usually in the form of fine clay, black shale and other minerals commonly associated with coal. The composition of the waste water associated with the production of coke by carbonization of coal indicates that it is high in phenols, ammonium and dissolved organics. The project does not delineate the specific composition of elements and specific organics in these waste waters. The waste streams studied were from individual processes within the refinery, coal mining, coal processing and coal utilization, the waste associated with each and the corresponding control measures.

Title: Sampling and Analytical Strategies for Compounds in Petroleum Refinery Streams

Authors: K. J. Bomba, E. C. Cavanaugh, J. C. Dickerman, S. L. Keil, T. P. Nelson, M. L. Own and D. D. Rosebrook

Performing Organization: Radian Corporation; Austin, TX 78766

Sponsoring Agency: EPA Industrial Environmental Research Laboratory
Research Triangle Park, NC 27711

Report No./Journal: Not Available

NTIS/GPO No.: Unknown Type of Report: Final; 1975

Abstract

This report presents as the principal objective the development of cost estimates for comprehensive sampling and analytical strategies for the examination of potentially hazardous components in five selected refinery effluents. Specifically, the streams to be analyzed are: (1) fugitive atomospheric emissions from atmospheric crude distillation; (2) aqueous condensate from the atmosphere crude still; (3) effluent water from the API separator; (4) tail gas from the sulphur recovery unit; and (5) atmospheric emissions from the fluid catalytic cracking regenerator.

Title: Current Practice in GC/MS Analysis of Organics in Water

Authors: R. G. Webb, A. W. Garrison, L. H. Keith and John M. McGuire

Performing Organization: Southeast Environmental Research Laboratory
College Station Rd., Athens, GA 30601

Sponsoring Agency: National Environmental Research Center, Office of Research and Monitoring, U. S. Environmental Protection Agency, Corvallis, OR 97330

Report No./Journal: EPA-R2-73-277

NTIS/GPO No.: EPA-R2-73-277 Type of Report: Government Technical, August, 1973

Abstract

This report discusses the analysis of waste water at the Southeast Environmental Research Laboratory utilizing the technique of gas chromatography/mass spectrometry. Procedures for extraction of aqueous media with solvents are reviewed and applied to the analysis of organic compounds in water from a petrochemical plant five-day lagoon effluent. Using a computerized data reduction system and a computerized spectrum matching program interfaced with a computer library of mass spectra, a total of 61 organic compounds was identified.

Title: Potentially Hazardous Emissions from the Extraction and Processing of Coal and Oil

Authors: H. E. Lebcwitz, S. Tam, G. Smithson, Jr., H. Nack, and J. Oxley; G. Cavanaugh, C. Burklin and J. Dickerman

Performing Organization: Battelle Columbus Laboratory and Radium Corporation

Sponsoring Agency: EPA, Office of Research and Development, NERC-RTP Control Systems Laboratory, Research Triangle Park, NC 27711

Report No./Journal: EPA-650/2-75-038

NTIS/GPO No.: PB-241-803 Type of Report: Government Task Final; 2-3-74

Abstract

This report lists the potentially hazardous materials which are known or suspected to be associated with air, water and solid waste from a refinery, a coke plant, a Lurgi high BTU gas process and the solvent coal process. From this study it is evident that available documents are not adequate to develop an accurate list of potentially hazardous emissions from these four processes. The recommendation is made for a detailed assessment of the processes, field sampling and analysis in order to identify the hazardous emissions more accurately.

This report includes a modular classification for potentially hazardous materials which has been proposed by EPA. The classification is divided as follows: acids and anhydrides, alcohols, amines, inorganic salts, carbonyl compounds, combustion gases, epoxides, ethers, halo-compounds, heterocyclic compounds, hydrocarbons, hydroperoxides, lactones, nitro compounds, nitrosoamines, ozonides, peroxides, phenols, polychlorinated polynuclears, polynuclear hydrocarbons, sulfur compounds, trace elements, organometallics, fine particulates and cyanides.

Title of Project: Hydrocarbons Emitted During Aeration of Refinery Waste Water (Air Stripping)

Principal Investigator: J. O. Ledbetter and J. W. Khim

Specialty: Civil Engineering

Performing Agency: University of Texas, School of Engineering, 200 W. 21st St., Austin, TX 78712

Supporting Agency: University of Texas

Agency's Number(s): Unknown

Project Period: 7/74 - 6/75 **Funds:** FY75 - Unknown

Summary

This project proposes to examine the amounts of hydrocarbons stripped from refinery waste water. Bench-scale studies will involve the measurements and identification of the hydrocarbon emissions from model activated sludge models.

Title: Analysis of Soluble Organic Constituents in Natural and Process Waters by High Pressure Liquid Chromatography

Authors: R. L. Jolley, W. W. Pitts, Jr., C. D. Scott, G. Jones, Jr. and J. E. Thompson

Performing Organization: Oak Ridge National Laboratory, Oak Ridge, Tennessee

Sponsoring Agency: Unknown

Report No./Journal: ERDA Research Abstracts, July 1975, 00847

NTIS/GPO No. Unknown **Type of Report:** Government Technical Publication

Abstract

This report presents the development of high pressure high resolution liquid chromatography at the Oak Ridge National Laboratory for detection, separation and analysis of soluble organics in a variety of waters of environmental concern. The separated constituents were subsequently identified by mass spectrometry.

Title of Project: The Chemistry of Tar Sand Bitumens

Principal Investigator: S. M. Dorrence

Performing Agency: U. S. Energy Research and Development Administration, Laramie Energy Research Center, Laramie, WY 82070

Supporting Agency: U. S. Energy Research and Development Administration

Agency's Number(s): Unknown

Project Period: 7/1/72 - 6/1/77 Funds: FY73 - $125,000
FY74 - $145,000
FY75 - $200,000

Summary

This program proposes to develop methods for *chemical characterization* of *oils*, *chars*, *gases* and *water contaminants* produced during laboratory and field experiments designed to develop *in situ* recovery of *tar sands*. Solvent extracted tar sand bitumens are being investigated to determine chemical composition and physical properties to establish how these parameters affect recovery. Gases and water soluble materials produced during recovery experiments will be analyzed to assess environmental impact.

Title of Project: In Situ Oil Recovery from Tar Sand Deposits: Chemical Studies (the commonly used short title is, Tar Sands Chemistry)

Principal Investigator: S. M. Dorrence

Speciality: Unknown

Performing Agency: U. S. ERDA; Laramie, Wyoming

Supporting Agency: U. S. ERDA; Washington, D. C.

Agency's Number(s): Unknown

Project Period: 7/1/72 - 6/30/84

Funds:
FY73 - $125,000
FY74 - $145,000
FY75 - $200,000
FY76 - $300,000

Summary

This project is involved with development of methods for chemical characterization of oils, tars, gases and waters produced during laboratory and field experiments designed to develop in situ recovery of tar sands. Solvent extracted tar sand bitumens are being investigated to determine chemical composition and physical properties to establish how these parameters affect recovery and to provide base line data to evaluate the extent to which produced oils are upgraded compared to original bitumens.

Title: Sampling Hot Springs for Radioactive and Trace Elements

Authors: Harold A. Wollenberg

Performing Organization: Lawrence Berkeley Laboratory, University
of California; Berkeley, CA 94720

Report No./Journal: Lawrence Berkeley Laboratory Report

NTIS/GPO No.: Unknown Type of Report: U. S. Government Annual

Abstract

The Lawrence Berkeley Laboratory is conducting a program to define the parameters for assessment of geothermal resources and to develop and evaluate techniques to measure these parameters. One of the major objectives of this program is the characterization of water samples for major and trace elements utilizing laboratory radiometry, x-ray fluorescence analysis (Si, Na, K. Ca, Al, Hg, S) and neutron activation analyses for trace elements. Under this program collection methods were devised to retain all solid material including particulates. Geothermal samples were taken for analysis from Big Sulphur, Hot Springs, Ruby Valley, Nevada; Leach Hot Springs, Nevada; and Kyle, Nevada.

APPENDIX B

ELEMENTAL CONSTITUENTS IN LIQUID AND SOLID EFFLUENTS FROM ENERGY-RELATED PROCESSES

Page

Part I: Samples from In Situ Oil-Shale Gasification (Tables B1-B3). 237

Part II: Samples from Low Btu Gasification of Rosebud Coal (Tables B4-B10) 240

Part III: Samples from In Situ Coal Gasification in Gillette, WY (Tables B11-B28). 247

Part IV: Samples from In Situ Coal Gasification in Hanna, WY (Tables B29-B48). 265

Table B1. ELEMENTAL CONCENTRATIONS IN LIQUID SAMPLE FROM 150 TON OIL-SHALE RETORT PROCESSING EXPERIMENT (LERC)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	0.026 ± .024	Fluorine	8 ± 2	Neodymium	<0.001	Strontium	0.75 ± .005
Antimony	0.24 ± .16	Gadolinium	0.001	Nickel	INT	Sulfur	MC
Arsenic	0.025 ± .005	Gallium	<0.002	Niobium	<0.001	Tantalum	0.003 ± .003
Barium	0.009 ± .001	Germanium	<0.001	Osmium	<0.001	Tellurium	<0.001
Beryllium	<0.001	Gold	<0.001	Palladium	<0.001	Terbium	<0.001
Bismuth	<0.001	Hafnium	<0.001	Phosphorus	0.8 ± .2	Thallium	<0.001
Boron	1.5 ± .5	Holmium	<0.001	Platinum	<0.001	Thorium	<0.001
Bromine	0.15 ± .05	Indium	[illegible]	Potassium	3 ± 0	Thulium	0.001
Cadmium	<0.001	Iodine	0.025 ± .005	Praseodymium	<0.001	Tin	0.002 ± .001
Calcium	2 ± 0	Iridium	<0.001	Rhenium	<0.001	Titanium	0.5 ± .3
Cerium	<0.001	Iron	3.5 ± .5	Rhodium	<0.001	Tungsten	0.002 ± 0
Cesium	<0.001	Lanthanum	<0.001	Rubidium	0.004 ± 0	Uranium	0.06 ± .01
Chlorine	MC	Lead	0.035 ± .005	Ruthenium	<0.001	Vandium	0.015 ± .005
Chromium	0.001 ± .001	Lithium	0.28 ± .21	Samarium	<0.001	Ytterbium	<0.001
Cobalt	0.01 ± 0	Lutetium	<0.001	Sandium	<0.001	Yttrium	<0.001
Copper	0.045 ± .025	Magnesium	4 ± 0	Selenium	0.003 ± 0	Zinc	0.02
Dysprosium	0.045 ± .025	Manganese	0.015 ± .005	Silicon	2.5 ± .5	Zirconium	0.04 ± .01
Erbium	<0.001	Mercury[b]	0.0009	Silver	<0.001		
Europium	<0.001	Molybdenum	0.3 ± 0	Sodium	MC		

[a] Detection limit was 0.001.

[b] Determined by flameless atomic absorption.

Table B2. ELEMENTAL CONCENTRATIONS IN DISCARDED CAVERN OIL SHALE FROM IN SITU OIL-SHALE PROCESSING (OOS)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	MC	Fluorine	MC	Neodymium	5 ± 0	Strontium	460 ± 0
Antimony	1 ± 0	Gadolinium	0.7 ± 0	Nickel	15 ± 0	Sulfur	MC
Arsenic	15 ± 2	Gallium	14 ± 1	Niobium	8 ± 2	Tantalum	<0.2
Barium	180 ± 10	Germanium	0.65 ± 0.2	Osmium	<0.2	Tellurium	<0.2
Beryllium	0.3 ± 0	Gold	<0.2	Palladium	<0.2	Terbium	0.55 ± .05
Bismuth	0.7 ± .3	Hafnium	<0.2	Phosphorus	MC	Thallium	<0.2
Boron	53 ± 18	Holmium	0.55 ± .05	Platinum	<0.2	Thorium	5 ± 1
Bromine	0.9 ± .1	Indium	[illegible]	Potassium	MC	Thulium	<0.2
Cadmium	≤0.8 ± .1	Iodine	0.5 ± 0.4	Praseodymium	3 ± 1	Tin	1.5 ± .5
Calcium	MC	Iridium	<0.2	Rhenium	<0.2	Titanium	MC
Cerium	55 ± 0	Iron	MC	Rhodium	<0.2	Tungsten	1.25 ± .75
Cesium	7 ± 2	Lanthanum	20 ± 0	Rubidium	125 ± 35	Uranium	3 ± 0
Chlorine	50 ± 14	Lead	19 ± 16	Ruthenium	<0.2	Vandium	135 ± 45
Chromium	125 ± 35	Lithium	160 ± 0	Samarium	1.5 ± 0.5	Ytterbium	<0.2
Cobalt	11 ± 4	Lutetium	<0.2	Sandium	25 ± 6	Yttrium	37 ± 0
Copper	48 ± 14	Magnesium	MC	Selenium	1 ± 0	Zinc	35 ± 32
Dysprosium	0.8 ± .1	Manganese	405 ± 170	Silicon	MC	Zirconium	110 ± 0
Erbium	0.3 ± 0	Mercury[b]	NA[c]	Silver	1.7 ± 1.3		
Europium	0.5 ± .1	Molybdenum	6 ± 3	Sodium	MC		

[a] Detection limit was 0.2.

[b] Determined by flameless atomic absorption.

[c] NA = not analyzed.

Table B3. ELEMENTAL CONCENTRATIONS IN BOILER BLOW-DOWN WATER FROM IN SITU OIL-SHALE PROCESSING (OOS)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	0.5 ± 0.1	Fluorine	MC	Neodymium	0.003 ± 0	Strontium	5 ± 0
Antimony	0.01 ± 0.05	Gadolinium	0.001	Nickel	0.08 ± 0	Sulfur	MC
Arsenic	2 ± 0	Gallium	0.015 ± .007	Niobium	0.003 ± .001	Tantalum	<0.001
Barium	0.5 ± 0.05	Germanium	0.015 ± .005	Osmium	<0.001	Tellurium	<0.001
Beryllium	<0.001	Gold	<0.001	Palladium	<0.001	Terbium	<0.001
Bismuth	<0.001	Hafnium	<0.001	Phosphorus	2.5 ± .5	Thallium	<0.001
Boron	1.7 ± 1.3	Holmium	<0.001	Platinum	<0.001	Thorium	<0.001
Bromine	0.3 ± 0	Indium	[illegible]	Potassium	MC	Thulium	<0.001
Cadmium	<0.001	Iodine	0.02 ± .01	Praseodymium	0.001 ± 0	Tin	0.040 ± .040
Calcium	MC	Iridium	<0.001	Rhenium	<0.001	Titanium	0.45 ± .05
Cerium	0.002 ± .001	Iron	5.5 ± 2.5	Rhodium	<0.001	Tungsten	<0.001
Cesium	0.01 ± 0	Lanthanum	0.001 ± 0	Rubidium	0.15 ± .05	Uranium	0.015 ± .005
Chlorine	MC	Lead	0.06 ± .03	Ruthenium	<0.001	Vandium	0.01 ± 0
Chromium	0.005 ± .002	Lithium	1.2 ± .8	Samarium	0.002 ± .001	Ytterbium	<0.001
Cobalt	0.01 ± 0	Lutetium	<0.001	Sandium	≤0.006 ± 0	Yttrium	0.002 ± 0
Copper	0.6 ± 0	Magnesium	MC	Selenium	0.014 ± .006	Zinc	0.12 ± .08
Dysprosium	<0.001	Manganese	0.06 ± .03	Silicon	MC	Zirconium	0.3 ± .1
Erbium	<0.001	Mercury[b]	0.001	Silver	<0.001		
Europium	0.001	Molybdenum	0.6 ± 0	Sodium	MC		

[a] Detection limit was 0.001.

[b] Determined by flameless atomic absorption.

Table B4. ELEMENTAL CONCENTRATIONS IN LIQUID CONDENSATE (-1L) FROM ROSEBUD COAL DURING LOW BTU COAL GASIFICATION (MERC)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	0.04 ± .02	Fluorine	0.08 ± .02	Neodymium	<0.004	Strontium	0.65 ± 0.05
Antimony	<0.004	Gadolinium	<0.004	Nickel	0.007 ± .003	Sulfur	2 ± 0
Arsenic	0.008 ± .001	Gallium	0.003 ± .003	Niobium	<0.004	Tantalum	<0.004
Barium	0.04 ± 0	Germanium	<0.004	Osmium	<0.004	Tellurium	<0.004
Beryllium	<0.004	Gold	<0.004	Palladium	<0.004	Terbium	<0.004
Bismuth	<0.004	Hafnium	<0.004	Phosphorus	0.3 ± .1	Thallium	<0.004
Boron	0.035 ± .005	Holmium	<0.004	Platinum	<0.004	Thorium	<0.004
Bromine	0.007 ± .003	Indium	[illegible]	Potassium	1.4 ± 0.8	Thulium	<0.004
Cadmium	<0.004	Iodine	0.003 ± .003	Praseodymium	<0.004	Tin	<0.004
Calcium	MC	Iridium	<0.004	Rhenium	<0.004	Titanium	0.08 ± .01
Cerium	0.003 ± 0	Iron	0.145 ± 0.06	Rhodium	<0.004	Tungsten	<0.004
Cesium	0.002 ± .002	Lanthanum	0.002 ± 0	Rubidium	0.005 ± .002	Uranium	<0.004
Chlorine	0.5 ± .2	Lead	0.025 ± .005	Ruthenium	<0.004	Vandium	0.002 ± .001
Chromium	0.025 ± .005	Lithium	0.095 ± .005	Samarium	<0.004	Ytterbium	<0.004
Cobalt	≤0.009 ± .009	Lutetium	<0.004	Scandium	≤0.007	Yttrium	0.002 ± .002
Copper	0.015 ± .005	Magnesium	5 ± 1	Selenium	≤0.005 ± .005	Zinc	0.035 ± .005
Dysprosium	<0.004	Manganese	0.02 ± 0	Silicon	0.6 ± 0	Zirconium	0.003 ± 0
Erbium	<0.004	Mercury[b]	<0.0015	Silver	<0.004		
Europium	<0.004	Molybdenum	0.009 ± .001	Sodium	≥10		

---

[a] Detection limit was 0.004.

[b] Determined by flameless atomic absorption.

Table B5. ELEMENTAL CONCENTRATIONS IN LIQUID CONDENSATE (-2L) FROM ROSEBUD COAL DURING LOW BTU COAL GASIFICATION (MERC)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	0.12 ± .07	Fluorine	0.13 ± .07	Neodymium	<.004	Strontium	0.6 ± .3
Antimony	<.004	Gadolinium	<.004	Nickel	0.015 ± .005	Sulfur	3 ± 3
Arsenic	0.014 ± .006	Gallium	0.005 ± .001	Niobium	<.004	Tantalum	<.004
Barium	0.07 ± 0.04	Germanium	≤0.003	Osmium	<.004	Tellurium	<.004
Beryllium	<.004	Gold	<.004	Palladium	<.004	Terbium	<.004
Bismuth	<.004	Hafnium	<.004	Phosphorus	0.55 ± .05	Thallium	<.004
Boron	0.07 ± .01	Holmium	<.004	Platinum	<.004	Thorium	≤0.004
Bromine	0.017 ± .012	Indium	<.004	Potassium	1.05 ± 1.0	Thulium	<.004
Cadmium	≤0.01	Iodine	≤0.002	Praseodymium	<.004	Tin	0.029 ± 0.021
Calcium	MC	Iridium	[illegible]	Rhenium	<.004	Titanium	0.25 ± .05
Cerium	0.003 ± .001	Iron	0.6 ± .1	Rhodium	<.004	Tungsten	<.004
Cesium	0.003 ± .001	Lanthanum	0.002 ± 0	Rubidium	0.006 ± .001	Uranium	≤0.004
Chlorine	0.6 ± .3	Lead	0.03 ± .02	Ruthenium	<.004	Vandium	0.002 ± .001
Chromium	0.015 ± .014	Lithium	0.1 ± 0	Samarium	<.004	Ytterbium	<.004
Cobalt	0.008 ± .001	Lutetium	<.004	Scandium	0.006 ± .001	Yttrium	0.001 ± .001
Copper	0.055 ± .015	Magnesium	7-	Selenium	0.005 ± .001	Zinc	0.06 ± .01
Dysprosium	<.004	Manganese	0.06 ± .03	Silicon	1.5 ± .5	Zirconium	0.002 ± .001
Erbium	<.004	Mercury[b]	<0.0015	Silver	<.004		
Europium	<.004	Molybdenum	0.008 ± .003	Sodium	8.5 ± 1.5		

[a] Detection limit was <0.004.

[b] Determined by flameless atomic absorption.

Table B6. ELEMENTAL CONCENTRATIONS IN LIQUID CONDENSATE (-3L) FROM ROSEBUD COAL DURING LOW BTU COAL GASIFICATION (MERC)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	0.045 ± .015	Fluorine	0.1 ± 0	Neodymium	<0.003	Strontium	0.45 ± .05
Antimony	<0.003	Gadolinium	<0.003	Nickel	0.055 ± .045	Sulfur	4 ± 2
Arsenic	0.035 ± .015	Gallium	0.001 ± .001	Niobium	<0.003	Tantalum	<0.003
Barium	0.055 ± .015	Germanium	0.001 ± .001	Osmium	<0.003	Tellurium	<0.003
Beryllium	<0.003	Gold	<0.003	Palladium	<0.003	Terbium	<0.003
Bismuth	<0.003	Hafnium	<0.003	Phosphorus	0.3 ± .1	Thallium	<0.003
Boron	0.035 ± .005	Holmium	<0.003	Platinum	<0.003	Thorium	<0.003
Bromine	0.011 ± .009	Indium	[illegible]	Potassium	2 ± 0	Thulium	<0.003
Cadmium	<0.003	Iodine	0.001 ± .001	Praseodymium	<0.003	Tin	0.006 ± .002
Calcium	<0.003	Iridium	<0.003	Rhenium	<0.003	Titanium	0.095 ± .005
Cerium	0.001 ± .001	Iron	0.35 ± .05	Rhodium	<0.003	Tungsten	<0.003
Cesium	0.002 ± .001	Lanthanum	0.002 ± .002	Rubidium	0.004 ± .003	Uranium	<0.003
Chlorine	1.5 ± .5	Lead	0.015 ± .005	Ruthenium	<0.003	Vandium	0.002 ± .001
Chromium	0.015 ± .005	Lithium	0.055 ± .005	Samarium	<0.003	Ytterbium	<0.003
Cobalt	0.004 ± .003	Lutetium	<0.003	Scandium	<0.003	Yttrium	0.001 ± .001
Copper	0.03 ± .01	Magnesium	MC	Selenium	0.002 ± .002	Zinc	0.03 ± 0
Dysprosium	<0.003	Manganese	0.05 ± .03	Silicon	0.75 ± .05	Zirconium	0.001 ± .001
Erbium	<0.003	Mercury[b]	<0.0015	Silver	≤0.001		
Europium	<0.003	Molybdenum	0.008 ± .002	Sodium	6 ± 3		

[a] Detection limit was <0.003.

[b] Determined by flameless atomic absorption.

Table B7. ELEMENTAL CONCENTRATIONS IN LIQUID CONDENSATE (-4L) FROM ROSEBUD COAL DURING LOW BTU COAL GASIFICATION (MERC)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	0.045 ± .035	Fluorine	0.15 ± .11	Neodymium	<0.002	Strontium	0.5 ± .44
Antimony	<0.002	Gadolinium	<0.002	Nickel	0.003 ± .002	Sulfur	2 ± 1
Arsenic	0.003 ± .002	Gallium	<0.002	Niobium	<0.002	Tantalum	<0.002
Barium	0.06 ± .05	Germanium	<0.002	Osmium	<0.002	Tellurium	<0.002
Beryllium	<0.002	Gold	<0.002	Palladium	<0.002	Terbium	<0.002
Bismuth	<0.002	Hafnium	<0.002	Phosphorus	0.3 ± .2	Thallium	<0.002
Boron	0.41 ± .4	Holmium	<0.002	Platinum	<0.002	Thorium	<0.002
Bromine	0.006 ± .004	Indium	[illegible]	Potassium	3.1 ± 3	Thulium	<0.002
Cadmium	<0.002	Iodine	<0.002	Praseodymium	<0.002	Tin	0.003 ± 0
Calcium	MC	Iridium	<0.002	Rhenium	<0.002	Titanium	0.012 ± .007
Cerium	0.001 ± .001	Iron	0.15 ± .05	Rhodium	<0.002	Tungsten	<0.002
Cesium	<0.002	Lanthanum	0.001 ± .001	Rubidium	0.003 ± .001	Uranium	<0.002
Chlorine	0.6 ± .6	Lead	0.015 ± .005	Ruthenium	<0.002	Vandium	0.001 ± .001
Chromium	0.013 ± .007	Lithium	0.125 ± .12	Samarium	<0.002	Ytterbium	<0.002
Cobalt	0.005 ± .004	Lutetium	<0.002	Scandium	≤0.002	Yttrium	0.001 ± .001
Copper	0.004 ± .003	Magnesium	MC	Selenium	<0.002	Zinc	0.045 ± .025
Dysprosium	<0.002	Manganese	0.4 ± .47	Silicon	1.6 ± 1.5	Zirconium	0.002 ± .001
Erbium	<0.002	Mercury[b]	<0.0015	Silver	<0.002		
Europium	<0.002	Molybdenum	0.007 ± .003	Sodium	7 ± 3		

[a] Detection limit was <0.002.

[b] Determined by flameless atomic absorption.

Table B8. ELEMENTAL CONCENTRATIONS IN LIQUID CONDENSATE (-5T) FROM
ROSEBUD COAL DURING LOW BTU COAL GASIFICATION (MERC)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	0.5 ± .45	Fluorine	0.6 ± .4	Neodymium	<0.02	Strontium	0.015 ± .005
Antimony	0.06 ± .02	Gadolinium	<0.02	Nickel	0.85 ± .05	Sulfur	MC
Arsenic	1 ± 0	Gallium	<0.02	Niobium	<0.02	Tantalum	0.3 ± .3
Barium	0.025 ± .005	Germanium	<0.02	Osmium	<0.02	Tellurium	<0.02
Beryllium	<0.02	Gold	<0.02	Palladium	<0.02	Terbium	<0.02
Bismuth	<0.02	Hafnium	<0.02	Phosphorus	0.07 ± .02	Thallium	<0.02
Boron	0.4 ± .2	Holmium	<0.02	Platinum	<0.02	Thorium	<0.02
Bromine	0.02 ± 0	Indium	[illegible]	Potassium	0.23 ± .17	Thulium	<0.02
Cadmium	<0.02	Iodine	<0.02	Praseodymium	<0.02	Tin	<0.02
Calcium	2.4 ± 1.7	Iridium	<0.02	Rhenium	<0.02	Titanium	0.1 ± 0
Cerium	<0.02	Iron	2.5 ± 1.5	Rhodium	<0.02	Tungsten	0.07 ± .07
Cesium	0.01 ± 0	Lanthanum	<0.02	Rubidium	0.05 ± .04	Uranium	<0.02
Chlorine	0.23 ± .17	Lead	0.1 ± 0	Ruthenium	<0.02	Vandium	0.033 ± .027
Chromium	0.06 ± .01	Lithium	0.020 ± .015	Samarium	<0.02	Ytterbium	<0.02
Cobalt	0.008 ± .002	Lutetium	<0.02	Scandium	0.02 ± .015	Yttrium	<0.02
Copper	0.2 ± .1	Magnesium	0.7 ± .4	Selenium	0.04 ± 0	Zinc	0.25 ± .2
Dysprosium	<0.02	Manganese	0.04 ± .02	Silicon	2.0 ± 1.1	Zirconium	0.02 ± .02
Erbium	<0.02	Mercury[b]	0.005	Silver	<0.02		
Europium	<0.02	Molybdenum	<0.02	Sodium	1.0 ± .9		

---

[a] Detection limit was <0.02.

[b] Determined by flameless atomic absorption.

Table B9. ELEMENTAL CONCENTRATIONS IN LIQUID CONDENSATE (-6T) FROM ROSEBUD COAL DURING LOW BTU COAL GASIFICATION (MERC)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	0.20 ± .12	Fluorine	0.3	Neodymium	<0.04	Strontium	0.04 ± .01
Antimony	≤0.04	Gadolinium	<0.04	Nickel	1.85 ± 1.15	Sulfur	MC
Arsenic	0.15 ± .05	Gallium	0.06 ± .06	Niobium	<0.04	Tantalum	0.7 ± .06
Barium	0.07 ± .03	Germanium	<0.04	Osmium	<0.04	Tellurium	<0.04
Beryllium	<0.04	Gold	<0.04	Palladium	<0.04	Terbium	<0.04
Bismuth	<0.04	Hafnium	<0.04	Phosphorus	0.3 ± .1	Thallium	<0.04
Boron	0.15 ± .05	Holmium	<0.04	Platinum	<0.04	Thorium	<0.04
Bromine	0.04 ± .01	Indium	[illegible]	Potassium	0.14 ± .06	Thulium	<0.04
Cadmium	<0.04	Iodine	<0.04	Praseodymium	<0.04	Tin	<0.04
Calcium	MC	Iridium	<0.04	Rhenium	<0.04	Titanium	0.15 ± .05
Cerium	<0.04	Iron	1.5 ± .5	Rhodium	<0.04	Tungsten	<0.04
Cesium	≤0.04	Lanthanum	<0.04	Rubidium	0.03 ± .01	Uranium	<0.04
Chlorine	1.0 ± .9	Lead	0.25 ± .05	Ruthenium	<0.04	Vandium	0.015 ± .005
Chromium	0.47 ± .43	Lithium	0.045 ± .005	Samarium	<0.04	Ytterbium	<0.04
Cobalt	0.015 ± .005	Lutetium	<0.04	Scandium	0.05 ± .02	Yttrium	<0.04
Copper	0.6 ± .4	Magnesium	2.0 ± 1.0	Selenium	0.08 ± .02	Zinc	0.5 ± .5
Dysprosium	<0.04	Manganese	0.020 ± .011	Silicon	1.5 ± .5	Zirconium	0.06 ± .06
Erbium	<0.04	Mercury[b]	0.005	Silver	<0.04		
Europium	<0.04	Molybdenum	<0.04	Sodium	0.2 ± .2		

[a] Detection limit was <0.04.

[b] Determined by flameless atomic absorption.

Table B10. ELEMENTAL CONCENTRATIONS IN LIQUID CONDENSATE (-7T) FROM ROSEBUD COAL DURING LOW BTU COAL GASIFICATION (MERC)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	1.6 ± 1.4	Fluorine	≈0.04 ± .01	Neodymium	<0.01	Strontium	0.008 ± .003
Antimony	≤0.03 ± .03	Gadolinium		Nickel	0.35 ± .15	Sulfur	MC
Arsenic	2.5 ± .5	Gallium	0.04 ± .01	Niobium	<0.01	Tantalum	0.15 ± .05
Barium	0.01 ± 0	Germanium	0.04 ± .02	Osmium	<0.01	Tellurium	<0.01
Beryllium	0.015 ± .005	Gold	<0.01	Palladium	<0.01	Terbium	<0.01
Bismuth	<0.01	Hafnium	<0.01	Phosphorus	0.05 ± .02	Thallium	<0.01
Boron	2 ± 1	Holmium	<0.01	Platinum	<0.01	Thorium	<0.01
Bromine	0.009 ± .002	Indium	[illegible]	Potassium	0.09 ± .01	Thulium	<0.01
Cadmium	<0.01	Iodine	<0.01	Praseodymium	<0.01	Tin	0.04 ± .02
Calcium	4.2 ± 4.0	Iridium	<0.01	Rhenium	<0.01	Titanium	0.13 ± .07
Cerium	<0.01	Iron	MC	Rhodium	<0.01	Tungsten	0.04 ± .01
Cesium	0.008 ± .001	Lanthanum	<0.01	Rubidium	0.007 ± .001	Uranium	<0.01
Chlorine	0.18 ± .12	Lead	0.06 ± .01	Ruthenium	<0.01	Vandium	0.060 ± .058
Chromium	0.09 ± .03	Lithium	0.020 ± .009	Samarium	<0.01	Ytterbium	<0.01
Cobalt	0.008 ± .003	Lutetium	<0.01	Scandium	0.006 ± .005	Yttrium	<0.01
Copper	0.075 ± .005	Magnesium	0.6 ± .1	Selenium	0.6 ± .05	Zinc	0.15 ± .05
Dysprosium	<0.01	Manganese	0.22 ± .18	Silicon	0.6 ± .4	Zirconium	0.025 ± .010
Erbium	<0.01	Mercury[b]	0.005	Silver	<0.01		
Europium	<0.01	Molybdenum	<0.01	Sodium	0.5 ± .1		

[a] Detection limit was <0.01.

[b] Determined by flameless atomic absorption.

Table B11. ELEMENTAL CONCENTRATIONS IN LIQUID SAMPLE (-1L) FROM DEWATERING WELL #5 PRIOR TO IN SITU COAL GASIFICATION (LLL)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	0.07 ± 0.03	Fluorine	≃0.15 ± 0.05	Neodymium	<0.001	Strontium	0.9 ± 0.1
Antimony	<0.001	Gadolinium	<0.001	Nickel	0.008 ± 0	Sulfur	<0.001
Arsenic	0.005 ± 0.002	Gallium	0.002 ± 0.002	Niobium	<0.001	Tantalum	<0.001
Barium	0.2 ± 0	Germanium	<0.001	Osmium	<0.001	Tellurium	<0.001
Beryllium	<0.001	Gold	<0.001	Palladium	<0.001	Terbium	<0.001
Bismuth	<0.001	Hafnium	<0.001	Phosphorus	0.14 ± 0.05	Thallium	<0.001
Boron	0.015 ± 0.014	Holmium	<0.001	Platinum	<0.001	Thorium	<0.001
Bromine	0.06 ± 0.02	Indium	[illegible]	Potassium	≥6	Thulium	<0.001
Cadmium	0.004 ± 0	Iodine	0.001 ± 0	Praseodymium	<0.001	Tin	<0.001
Calcium	MC	Iridium	<0.001	Rhenium	<0.001	Titanium	0.22 ± 0.18
Cerium	<0.001	Iron	0.15 ± 0.05	Rhodium	<0.001	Tungsten	<0.001
Cesium	0.001 ± 0	Lanthanum	<0.001	Rubidium	0.006 ± 0.001	Uranium	<0.001
Chlorine	3 ± 2	Lead	0.007 ± 0.001	Ruthenium	<0.001	Vandium	0.001 ± 0
Chromium	0.015 ± 0.005	Lithium	0.2 ± 0	Samarium	<0.001	Ytterbium	<0.001
Cobalt	0.002 ± 0	Lutetium	<0.001	Sandium	0.002 ± 0	Yttrium	<0.001
Copper	0.04 ± 0.01	Magnesium	MC	Selenium	<0.001	Zinc	0.075 ± 0.025
Dysprosium	<0.001	Manganese	0.3 ± 0	Silicon	4 ± 1	Zirconium	0.001 ± 0
Erbium	<0.001	Mercury[b]	<0.009	Silver	0.002 ± 0.002		
Europium	<0.001	Molybdenum	0.025 ± 0.005	Sodium	3.5 ± 0.5		

[a] Detection limit was 0.001.

[b] Determined by flameless atomic absorption.

Table B12. ELEMENTAL CONCENTRATIONS IN A BLEND LIQUID SAMPLE (-2L) FROM DEWATERING WELLS #1 AND 6 (LLL)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	0.07 ± 0.3	Fluorine	≃0.3 ± 0.05	Neodymium	<0.004	Strontium	2 ± 1
Antimony	0.003 ± 0.003	Gadolinium	<0.004	Nickel	0.035 ± 0.005	Sulfur	7 ± 1
Arsenic	0.004 ± 0.002	Gallium	0.002 ± 0.002	Niobium	0.002 ± 0.002	Tantalum	<0.004
Barium	0.1 ± 0	Germanium	<0.004	Osmium	<0.004	Tellurium	<0.004
Beryllium	<0.004	Gold	<0.004	Palladium	<0.004	Terbium	<0.004
Bismuth	<0.004	Hafnium	<0.004	Phosphorus	0.1 ± 0	Thallium	<0.004
Boron	0.07 ± 0.01	Holmium	<0.004	Platinum	<0.004	Thorium	<0.004
Bromine	0.25 ± 0.05	Indium	[illegible]	Potassium	MC	Thulium	<0.004
Cadmium	0.009 ± 0.009	Iodine	0.003 ± 0.003	Praseodymium	<0.004	Tin	<0.004
Calcium	MC	Iridium	<0.004	Rhenium	<0.004	Titanium	0.08 ± 0.02
Cerium	<0.004	Iron	0.6 ± 0.4	Rhodium	<0.004	Tungsten	0.01 ± 0.01
Cesium	0.002 ± 0	Lanthanum	<0.004	Rubidium	0.004 ± 0	Uranium	<0.004
Chlorine	3.5 ± 1.5	Lead	0.02 ± 0	Ruthenium	<0.004	Vandium	0.001 ± 0.001
Chromium	0.04 ± 0.01	Lithium	0.15 ± 0.06	Samarium	<0.004	Ytterbium	<0.004
Cobalt	0.001 ± 0	Lutetium	<0.004	Sandium	0.007 ± 0.002	Yttrium	0.001 ± 0.001
Copper	0.04 ± 0.01	Magnesium	MC	Selenium	0.004 ± 0.004	Zinc	0.1 ± 0
Dysprosium	<0.004	Manganese	0.25 ± 0.05	Silicon	MC	Zirconium	0.008 ± 0.002
Erbium	<0.004	Mercury[b]	<0.009	Silver	<0.004		
Europium	<0.004	Molybdenum	0.085 ± 0.005	Sodium	MC		

[a] Detection limit was 0.004.

[b] Determined by flameless atomic absorption.

Table B13. ELEMENTAL CONCENTRATIONS IN PROCESS WATER SAMPLE (-3L) FROM IN SITU COAL GASIFICATION (LLL)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	MC	Fluorine	≈1 ± 0	Neodymium	<0.004	Strontium	0.06 ± 0.04
Antimony	<0.004	Gadolinium	<0.004	Nickel	0.15 ± 0.05	Sulfur	MC
Arsenic	0.04 ± 0.02	Gallium	0.007 ± 0.002	Niobium	<0.004	Tantalum	<0.004
Barium	0.25 ± 0.05	Germanium	0.004 ± 0.004	Osmium	<0.004	Tellurium	<0.004
Beryllium	0.004	Gold	<0.004	Palladium	<0.004	Terbium	<0.004
Bismuth	<0.004	Hafnium	<0.004	Phosphorus	0.4 ± 0.1	Thallium	<0.004
Boron	0.09 ± 0.01	Holmium	<0.004	Platinum	<0.004	Thorium	<0.004
Bromine	0.006 ± 0.003	Indium	[illegible]	Potassium	5 ± 1	Thulium	<0.004
Cadmium	<0.004	Iodine	<0.004	Praseodymium	<0.004	Tin	<0.004
Calcium	MC	Iridium	<0.004	Rhenium	<0.004	Titanium	0.6 ± 0.4
Cerium	0.004 ± 0.004	Iron	4.5 ± 3.5	Rhodium	<0.004	Tungsten	<0.004
Cesium	0.004 ± 0.003	Lanthanum	0.002 ± 0.002	Rubidium	0.006 ± 0.002	Uranium	<0.004
Chlorine	2 ± 1	Lead	<0.04 ± 0.02	Ruthenium	<0.004	Vandium	0.013 ± 0.007
Chromium	0.07 ± 0.03	Lithium	0.085 ± 0.005	Samarium	<0.004	Ytterbium	<0.004
Cobalt	0.003 ± 0	Lutetium	<0.004	Sandium	0.013 ± 0.006	Yttrium	<0.004
Copper	0.9 ± 0.1	Magnesium	6 ± 2	Selenium	0.06 ± 0.04	Zinc	0.07 ± 0.3
Dysprosium	<0.004	Manganese	0.35 ± 0.25	Silicon	MC	Zirconium	0.01 ± 0
Erbium	<0.004	Mercury[b]	0.010	Silver	<0.004		
Europium	<0.004	Molybdenum	0.08 ± 0.02	Sodium	MC		

[a] Detection limit was <0.004.

[b] Determined by flameless atomic absorption.

Table B14. ELEMENTAL CONCENTRATIONS IN PROCESS TAR (-4T) FROM IN SITU COAL GASIFICATION (LLL)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	MC	Fluorine	≃ 4 ± 1	Neodymium	<0.04	Strontium	1 ± 0
Antimony	<0.04	Gadolinium	<0.04	Nickel	0.9 ± 0.1	Sulfur	MC
Arsenic	1.8 ± 1.2	Gallium	0.15 ± 0.05	Niobium	<0.04	Tantalum	<0.04
Barium	1.7 ± 1.3	Germanium	<0.04	Osmium	<0.04	Tellurium	<0.04
Beryllium	0.005 ± 0.005	Gold	<0.04	Palladium	<0.04	Terbium	<0.04
Bismuth	0.3 ± 0.3	Hafnium	<0.04	Phosphorus	1.5 ± 0.5	Thallium	0.1 ± 0.1
Boron	0.48 ± 0.42	Holmium	<0.04	Platinum	<0.04	Thorium	≤0.03 ± 0.03
Bromine	0.04 ± 0.02	Indium	[illegible]	Potassium	MC	Thulium	<0.04
Cadmium	0.2 ± 0.1	Iodine	<0.04	Praseodymium	<0.04	Tin	0.06 ± 0
Calcium	MC	Iridium	<0.04	Rhenium	<0.04	Titanium	5 ± 2
Cerium	0.03 ± 0	Iron	MC	Rhodium	<0.04	Tungsten	<0.04
Cesium	0.06 ± 0.04	Lanthanum	0.02 ± 0.02	Rubidium	0.35 ± 0.05	Uranium	≤0.04 ± 0.04
Chlorine	12.5 ± 12.0	Lead	<0.04	Ruthenium	<0.04	Vandium	0.06 ± 0.03
Chromium	0.7 ± 0.3	Lithium	0.7 ± 0.1	Samarium	<0.04	Ytterbium	<0.04
Cobalt	0.08 ± 0.02	Lutetium	<0.04	Sandium	0.06 ± 0.02	Yttrium	<0.04
Copper	2 ± 0	Magnesium	MC	Selenium	0.015 ± 0.05	Zinc	0.06 ± 0.04
Dysprosium	<0.04	Manganese	1.5 ± 0.5	Silicon	MC	Zirconium	0.06 ± 0.04
Erbium	<0.04	Mercury[b]	<0.230	Silver	<0.04		
Europium	<0.04	Molybdenum	<0.04	Sodium	MC		

[a] Detection limit was <0.04.

[b] Determined by flameless atomic absorption.

Table B15. ELEMENTAL CONCENTRATIONS IN WELL WATER FROM PERM #5 (-5L) IN SITU COAL GASIFICATION EXPERIMENT (LLL)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	0.15 ± 0.05	Fluorine	≈0.5 ± 0.1	Neodymium	<0.001	Strontium	2.5 ± 0.5
Antimony	0.001 ± 0.001	Gadolinium	<0.001	Nickel	0.03 ± 0.01	Sulfur	MC
Arsenic	0.003 ± 0.002	Gallium	0.001 ± 0.001	Niobium	<0.001	Tantalum	<0.001
Barium	0.07 ± 0.01	Germanium	<0.001	Osmium	<0.001	Tellurium	<0.001
Beryllium	<0.001	Gold	<0.001	Palladium	<0.001	Terbium	<0.001
Bismuth	<0.001	Hafnium	<0.001	Phosphorus	0.15 ± 0.05	Thallium	<0.001
Boron	0.06 ± 0	Holmium	<0.001	Platinum	<0.001	Thorium	<0.001
Bromine	0.023 ± 0.024	Indium	[illegible]	Potassium	MC	Thulium	<0.001
Cadmium	0.02 ± 0.01	Iodine	0.001 ± 0.001	Praseodymium	<0.001	Tin	<0.001
Calcium	MC	Iridium	<0.001	Rhenium	<0.001	Titanium	0.22 ± 0.17
Cerium	0.002 ± 0.002	Iron	0.7 ± 0.3	Rhodium	<0.001	Tungsten	<0.001
Cesium	0.003 ± 0.002	Lanthanum	0.001 ± 0.001	Rubidium	0.012 ± 0.008	Uranium	<0.001
Chlorine	1.7 ± 1.1	Lead	0.05 ± 0.01	Ruthenium	<0.001	Vandium	0.001 ± 0.001
Chromium	0.025 ± 0.005	Lithium	0.2 ± 0	Samarium	<0.001	Ytterbium	<0.001
Cobalt	0.002 ± 0	Lutetium	<0.001	Sandium	0.005 ± 0.006	Yttrium	<0.001
Copper	0.04 ± 0.01	Magnesium	MC	Selenium	0.002 ± 0.001	Zinc	0.17 ± 0.13
Dysprosium	<0.001	Manganese	1.6 ± 1.4	Silicon	5 ± 3	Zirconium	<0.001
Erbium	<0.001	Mercury[b]	<0.009	Silver	0.001 ± 0.001		
Europium	<0.001	Molybdenum	0.01 ± 0	Sodium	MC		

[a] Detection limit was 0.001.

[b] Determined by flameless atomic absorption.

Table B16. ELEMENTAL CONCENTRATIONS IN WELL WATER - EW4 (-8L) FROM IN SITU COAL GASIFICATION EXPERIMENT (LLL)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	0.028 ± .022	Fluorine	≈0.25 ± .15	Neodymium	<0.004	Strontium	0.6 ± .3
Antimony	0.004 ± .001	Gadolinium	<0.004	Nickel	0.01 ± 0	Sulfur	MC
Arsenic	≤0.002	Gallium	0.003 ± .001	Niobium	<0.004	Tantalum	<0.004
Barium	0.05 ± .02	Germanium	<0.004	Osmium	<0.004	Tellurium	<0.004
Beryllium	<0.004	Gold	<0.004	Palladium	<0.004	Terbium	<0.004
Bismuth	<0.004	Hafnium	<0.004	Phosphorus	0.24 ± .2	Thallium	<0.004
Boron	0.08 ± .02	Holmium	<0.004	Platinum	<0.004	Thorium	<0.004
Bromine	0.005 ± .004	Indium	I	Potassium	5 ± 3	Thulium	<0.004
Cadmium	≤0.01	Iodine	<0.004	Praseodymium	<0.004	Tin	<0.004
Calcium	MC	Iridium	<0.004	Rhenium	<0.004	Titanium	0.09 ± .01
Cerium	0.002 ± 0	Iron	7 ± 1	Rhodium	<0.004	Tungsten	<0.004
Cesium	≤0.002	Lanthanum	<0.004	Rubidium	≤0.002	Uranium	<0.004
Chlorine	5 ± 3	Lead	≤0.01	Ruthenium	<0.004	Vandium	≤0.001
Chromium	0.006 ± .003	Lithium	0.25 ± .05	Samarium	<0.004	Ytterbium	<0.004
Cobalt	≤0.005	Lutetium	<0.004	Scandium	≤0.003	Yttrium	≤0.001
Copper	0.017 ± .012	Magnesium	MC	Selenium	≤0.005	Zinc	0.06 ± .04
Dysprosium	<0.004	Manganese	0.07 ± .06	Silicon	3 ± 2	Zirconium	≤0.003
Erbium	<0.004	Mercury[b]	0.039	Silver	<0.004		
Europium	<0.004	Molybdenum	≤0.009	Sodium	MC		

---

[a] Detection limit was 0.004.

[b] Determined by flameless atomic absorption.

Table B17. ELEMENTAL CONCENTRATIONS IN WELL WATER - EW5 (-9L) FROM IN SITU COAL GASIFICATION EXPERIMENT (LLL)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	0.02 ± .01	Fluorine	≈0.1 ± .05	Neodymium	<0.003	Strontium	0.65 ± .05
Antimony	≤0.002	Gadolinium	<0.003	Nickel	0.007 ± .002	Sulfur	2 ± 0
Arsenic	0.003 ± .002	Gallium	≤0.001	Niobium	<0.003	Tantalum	<0.003
Barium	0.07 ± .04	Germanium	<0.003	Osmium	<0.003	Tellurium	<0.003
Beryllium	<0.003	Gold	<0.003	Palladium	<0.003	Terbium	<0.003
Bismuth	<0.003	Hafnium	<0.003	Phosphorus	0.06 ± .02	Thallium	<0.003
Boron	0.04 ± .02	Holmium	<0.003	Platinum	<0.003	Thorium	<0.003
Bromine	0.005 ± .001	Indium	[illegible]	Potassium	2 ± 0	Thulium	<0.003
Cadmium	<0.003	Iodine	≤0.002	Praseodymium	0.001 ± .001	Tin	≤0.004
Calcium	MC	Iridium	<0.003	Rhenium	<0.003	Titanium	0.2 ± 0
Cerium	0.002 ± 0	Iron	MC	Rhodium	<0.003	Tungsten	<0.003
Cesium	≤0.001	Lanthanum	0.001 ± .001	Rubidium	0.001 ± .001	Uranium	<0.003
Chlorine	3 ± 0	Lead	≤0.008	Ruthenium	<0.003	Vandium	<0.001
Chromium	0.002 ± 0	Lithium	0.11 ± .1	Samarium	<0.003	Ytterbium	<0.003
Cobalt	≤0.004	Lutetium	<0.003	Scandium	≤0.002	Yttrium	0.001 ± 0
Copper	0.003 ± 0	Magnesium	6 ± 2	Selenium	≤0.003	Zinc	0.02 ± .01
Dysprosium	<0.003	Manganese	0.7 ± .2	Silicon	2.5 ± .5	Zirconium	0.006 ± .004
Erbium	<0.003	Mercury[b]	0.067	Silver	<0.003		
Europium	<0.003	Molybdenum	≤0.007	Sodium	MC		

---

[a] Detection limit was 0.003.

[b] Determined by flameless atomic absorption.

Table B18. ELEMENTAL CONCENTRATIONS IN WELL WATER - DW#4 (-10L) FROM IN SITU COAL GASIFICATION EXPERIMENT (LLL)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	0.22 ± .2	Fluorine	≈0.8 ± .2	Neodymium	<0.004	Strontium	0.55 ± .25
Antimony	<0.004	Gadolinium	<0.004	Nickel	0.015 ± .005	Sulfur	MC
Arsenic	<0.004	Gallium	0.003 ± .001	Niobium	<0.004	Tantalum	<0.004
Barium	0.07 ± .02	Germanium	≤0.002	Osmium	<0.004	Tellurium	<0.004
Beryllium	<0.004	Gold	<0.004	Palladium	<0.004	Terbium	<0.004
Bismuth	<0.004	Hafnium	<0.004	Phosphorus	0.08 ± .02	Thallium	<0.004
Boron	0.45 ± .05	Holmium	<0.004	Platinum	<0.004	Thorium	<0.004
Bromine	0.25 ± .05	Indium	[illegible]	Potassium	MC	Thulium	<0.004
Cadmium	<0.004	Iodine	0.02 ± 0	Praseodymium	<0.004	Tin	≤0.009
Calcium	MC	Iridium	<0.004	Rhenium	<0.004	Titanium	0.25 ± .05
Cerium	≤0.003	Iron	MC	Rhodium	<0.004	Tungsten	<0.004
Cesium	≤0.002	Lanthanum	≤0.002	Rubidium	0.04 ± .02	Uranium	<0.004
Chlorine	4.5 ± 2.5	Lead	≤0.01	Ruthenium	<0.004	Vandium	0.01 ± 0
Chromium	0.008 ± .002	Lithium	0.4 ± 0	Samarium	<0.004	Ytterbium	<0.004
Cobalt	0.02 ± .01	Lutetium	<0.004	Scandium	≤0.004	Yttrium	≤0.001
Copper	0.009 ± .001	Magnesium	MC	Selenium	0.007 ± .002	Zinc	0.03 ± .01
Dysprosium	<0.004	Manganese	0.45 ± .05	Silicon	2.5 ± .5	Zirconium	0.004 ± .001
Erbium	<0.004	Mercury[b]	0.070	Silver	<0.004		
Europium	<0.004	Molybdenum	≤.005	Sodium	MC		

[a] Detection limit was 0.004.

[b] Determined by flameless atomic absorption.

Table B19. ELEMENTAL CONCENTRATIONS IN WELL WATER - DW#5 (-11L) FROM IN SITU COAL GASIFICATION EXPERIMENT (LLL)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	0.02 ± .01	Fluorine	≈0.8 ± .1	Neodymium	0.006	Strontium	1 ± 0
Antimony	0.002	Gadolinium	<0.006	Nickel	0.03 ± .02	Sulfur	MC
Arsenic	0.005 ± .001	Gallium	0.003 ± .003	Niobium	<0.006	Tantalum	<0.006
Barium	0.13 ± .07	Germanium	<0.006	Osmium	<0.006	Tellurium	<0.006
Beryllium	<0.006	Gold	<0.006	Palladium	<0.006	Terbium	<0.006
Bismuth	<0.006	Hafnium	<0.006	Phosphorus	0.095 ± .005	Thallium	<0.006
Boron	0.1 ± 0	Holmium	<0.006	Platinum	<0.006	Thorium	<0.006
Bromine	0.07 ± .02	Indium	[illegible]	Potassium	1.5 ± .5	Thulium	<0.006
Cadmium	<0.006	Iodine	<0.006	Praseodymium	<0.006	Tin	<0.006
Calcium	MC	Iridium	<0.006	Rhenium	<0.006	Titanium	0.25 ± .05
Cerium	≤0.002	Iron	MC	Rhodium	<0.006	Tungsten	<0.006
Cesium	≤0.002	Lanthanum	<0.006	Rubidium	0.008 ± .002	Uranium	<0.006
Chlorine	MC	Lead	≤0.01	Ruthenium	<0.006	Vandium	0.001 ± .001
Chromium	0.005 ± .001	Lithium	0.09 ± .01	Samarium	<0.006	Ytterbium	<0.006
Cobalt	≤0.006	Lutetium	<0.006	Scandium	≤0.004	Yttrium	<0.006
Copper	0.015 ± .005	Magnesium	7.5 ± .5	Selenium	≤0.005	Zinc	0.02 ± .01
Dysprosium	<0.006	Manganese	0.3 ± 0	Silicon	3 ± 1	Zirconium	0.004 ± .001
Erbium	<0.006	Mercury[b]	0.015	Silver	≤0.003		
Europium	<0.006	Molybdenum	≤0.007	Sodium	MC		

[a] Detection limit was 0.006.

[b] Determined by flameless atomic absorption.

Table B20. ELEMENTAL CONCENTRATIONS IN WATER SAMPLE FROM EM-1 WELL (-12L) AFTER IN SITU COAL GASIFICATION (LLL)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	0.09 ± .02	Fluorine	0.9 ± .1	Neodymium	<0.009	Strontium	2 ± 0
Antimony	<0.009	Gadolinium	<0.009	Nickel	0.015 ± .005	Sulfur	MC
Arsenic	0.006 ± 0	Gallium	≤0.008	Niobium	<0.009	Tantalum	<0.009
Barium	0.09 ± 0	Germanium	<0.009	Osmium	<0.009	Tellurium	<0.009
Beryllium	<0.009	Gold	<0.009	Palladium	<0.009	Terbium	<0.009
Bismuth	<0.009	Hafnium	<0.009	Phosphorus	0.18 ± .17	Thallium	<0.009
Boron	0.025 ± .005	Holmium	<0.009	Platinum	<0.009	Thorium	<0.009
Bromine	0.02 ± .01	Indium	[illegible]	Potassium	5.5 ± .5	Thulium	<0.009
Cadmium	<0.009	Iodine	0.006 ± 0	Praseodymium	<0.009	Tin	<0.009
Calcium	MC	Iridium	<0.009	Rhenium	<0.009	Titanium	0.1 ± 0
Cerium	0.008 ± .001	Iron	0.45 ± .05	Rhodium	<0.009	Tungsten	<0.03
Cesium	≤0.006	Lanthanum	<0.007	Rubidium	0.015 ± .005	Uranium	<0.009
Chlorine	2 ± 0	Lead	0.09 ± .01	Ruthenium	<0.009	Vandium	0.003 ± 0
Chromium	0.025 ± .005	Lithium	0.1	Samarium	<0.009	Ytterbium	<0.009
Cobalt	0.02 ± .01	Lutetium	<0.009	Scandium	0.01 ± .005	Yttrium	<0.004
Copper	0.11 ± .09	Magnesium	MC	Selenium	≤0.02	Zinc	0.075 ± .025
Dysprosium	<0.009	Manganese	0.3 ± 0	Silicon	3.5 ± .5	Zirconium	0.014 ± .006
Erbium	<0.009	Mercury[b]	<0.23	Silver	<0.009		
Europium	<0.009	Molybdenum	0.06 ± .02	Sodium	MC		

---

[a] Detection limit was 0.009.

[b] Determined by flameless atomic absorption.

Table B21. ELEMENTAL CONCENTRATIONS IN WATER SAMPLE FROM EM-4 WELL (-13L) AFTER IN SITU COAL GASIFICATION

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	0.06 ± .03	Fluorine	≃4	Neodymium	<0.005	Strontium	3.5 ± 1.5
Antimony	<0.005	Gadolinium	<0.005	Nickel	0.035 ± .005	Sulfur	MC
Arsenic	0.006 ± .003	Gallium	0.006 ± .002	Niobium	<0.005	Tantalum	<0.005
Barium	0.19 ± .11	Germanium	<0.005	Osmium	<0.005	Tellurium	<0.005
Beryllium	<0.005	Gold	<0.005	Palladium	<0.005	Terbium	<0.005
Bismuth	<0.005	Hafnium	<0.005	Phosphorus	0.15 ± .05	Thallium	<0.005
Boron	0.03 ± .02	Holmium	<0.005	Platinum	<0.005	Thorium	<0.005
Bromine	0.09 ± .01	Indium	[illegible]	Potassium	MC	Thulium	<0.005
Cadmium	<0.005	Iodine	0.007 ± .004	Praseodymium	<0.005	Tin	<0.005
Calcium	MC	Iridium	<0.005	Rhenium	<0.005	Titanium	0.09 ± .01
Cerium	0.005 ± .001	Iron	1.5 ± .5	Rhodium	<0.005	Tungsten	<0.005
Cesium	0.005 ± .001	Lanthanum	0.004 ± .001	Rubidium	0.01 ± 0	Uranium	<0.005
Chlorine	6 ± 1	Lead	0.05 ± .02	Ruthenium	<0.005	Vandium	0.002 ± .001
Chromium	0.015 ± .005	Lithium	0.1 ± 0	Samarium	<0.005	Ytterbium	<0.005
Cobalt	<0.01	Lutetium	<0.005	Scandium	0.015 ± .005	Yttrium	0.003 ± .001
Copper	0.06 ± .02	Magnesium	MC	Selenium	0.009 ± .001	Zinc	0.15 ± .05
Dysprosium	<0.005	Manganese	0.65 ± .05	Silicon	7 ± 2	Zirconium	0.007 ± .002
Erbium	<0.005	Mercury[b]	<0.009	Silver	<0.006		
Europium	<0.005	Molybdenum	0.02 ± .02	Sodium	MC		

[a] Detection limit was 0.005.

[b] Determine by flameless atomic absorption.

Table B22. ELEMENTAL CONCENTRATIONS IN WATER SAMPLE FROM EM-2 WELL (-14L) AFTER IN SITU COAL GASIFICATION

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	0.07 ± .03	Fluorine	≃1	Neodymium	<0.005	Strontium	2 ± 0
Antimony	<0.005	Gadolinium	<0.005	Nickel	0.02 ± 0	Sulfur	MC
Arsenic	0.009 ± .001	Gallium	0.007 ± .002	Niobium	<0.005	Tantalum	<0.005
Barium	0.15 ± .05	Germanium	<0.005	Osmium	<0.005	Tellurium	<0.005
Beryllium	<0.005	Gold	<0.005	Palladium	<0.005	Terbium	<0.005
Bismuth	<0.005	Hafnium	<0.005	Phosphorus	0.13 ± .07	Thallium	<0.005
Boron	0.015 ± .005	Holmium	<0.005	Platinum	<0.005	Thorium	<0.005
Bromine	0.06 ± .02	Indium	[illegible]	Potassium	7 ± 2	Thulium	<0.005
Cadmium	<0.005	Iodine	0.005 ± .001	Praseodymium	<0.005	Tin	<0.005
Calcium	MC	Iridium	<0.005	Rhenium	<0.005	Titanium	0.075 ± .005
Cerium	0.006 ± .002	Iron	0.6 ± .3	Rhodium	<0.005	Tungsten	0.03
Cesium	0.005 ± .001	Lanthanum	<0.005	Rubidium	0.007 ± .001	Uranium	<0.005
Chlorine	3.5 ± 1.5	Lead	0.03 ± .01	Ruthenium	<0.005	Vandium	0.002 ± .001
Chromium	0.03 ± 0	Lithium	0.2 ± 0	Samarium	<0.005	Ytterbium	<0.005
Cobalt	0.009 ± .001	Lutetium	<0.005	Scandium	0.025 ± .005	Yttrium	<0.005
Copper	0.5 ± .45	Magnesium	MC	Selenium	0.009 ± .001	Zinc	0.06 ± .01
Dysprosium	<0.005	Manganese	0.3 ± 0	Silicon	3 ± 2	Zirconium	0.006 ± .002
Erbium	<0.005	Mercury[b]	<0.009	Silver	<0.005		
Europium	<0.005	Molybdenum	0.05 ± .01	Sodium	MC		

[a] Detection limit was 0.005.

[b] Determined by flameless atomic absorption.

Table B23. ELEMENTAL CONCENTRATIONS IN TAR SAMPLE (-15T) FROM PRODUCTION WELL #1 AFTER IN SITU COAL GASIFICATION (LLL)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	>15	Fluorine	≃4	Neodymium	0.06 ± .01	Strontium	19 ± 0
Antimony	0.2 ± .1	Gadolinium	0.04 ± .04	Nickel	2 ± 1	Sulfur	MC
Arsenic	0.2 ± .1	Gallium	0.07 ± .02	Niobium	0.05 ± .02	Tantalum	<0.01
Barium	4 ± 0	Germanium	0.05 ± 0	Osmium	<0.01	Tellurium	<0.01
Beryllium	<0.01	Gold	<0.01	Palladium	<0.01	Terbium	<0.01
Bismuth	0.05 ± .01	Hafnium	<0.01	Phosphorus	MC	Thallium	≤0.02
Boron	0.3 ± 0	Holmium	<0.01	Platinum	<0.01	Thorium	≤0.01
Bromine	0.09 ± 0	Indium	[illegible]	Potassium	42 ± 28	Thulium	<0.01
Cadmium	5.5 ± .5	Iodine	0.11 ± .09	Praseodymium	0.015 ± .005	Tin	1.5 ± .5
Calcium	MC	Iridium	<0.01	Rhenium	<0.01	Titanium	MC
Cerium	0.07 ± .03	Iron	MC	Rhodium	<0.01	Tungsten	<0.01
Cesium	0.035 ± .005	Lanthanum	0.03 ± .01	Rubidium	0.3 ± .1	Uranium	≤0.01
Chlorine	13 ± 0	Lead	65 ± 4	Ruthenium	<0.01	Vandium	0.5 ± .1
Chromium	1 ± 0	Lithium	0.45 ± .25	Samarium	0.035 ± .005	Ytterbium	<0.01
Cobalt	0.85 ± .15	Lutetium	<0.01	Scandium	≤0.03	Yttrium	0.04 ± .02
Copper	MC	Magnesium	MC	Selenium	0.15 ± .06	Zinc	MC
Dysprosium	<0.01	Manganese	MC	Silicon	MC	Zirconium	0.06 ± .05
Erbium	<0.01	Mercury[b]	<0.23	Silver	0.06 ± 0		
Europium	0.02 ± 0	Molybdenum	0.4 ± .1	Sodium	>39		

[a] Detection limit was 0.01.

[b] Determined by flameless atomic absorption.

Table B24. ELEMENTAL CONCENTRATIONS IN WATER SAMPLE (-16L) FROM WELL DW-4 FROM *IN SITU* COAL GASIFICATION EXPERIMENT (LLL)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	0.04 ± .04	Fluorine	≃3	Neodymium	<0.008	Strontium	5 ± 1
Antimony	<0.008	Gadolinium	<0.008	Nickel	0.05 ± .01	Sulfur	MC
Arsenic	0.006 ± .001	Gallium	0.007 ± 0	Niobium	<0.008	Tantalum	<0.008
Barium	0.13 ± .06	Germanium	<0.008	Osmium	<0.008	Tellurium	<0.008
Beryllium	<0.008	Gold	<0.008	Palladium	<0.008	Terbium	<0.008
Bismuth	<0.008	Hafnium	<0.008	Phosphorus	0.6 ± .4	Thallium	<0.008
Boron	0.12 ± .08	Holmium	<0.008	Platinum	<0.008	Thorium	<0.008
Bromine	0.05 ± 0	Indium	[illegible]	Potassium	MC	Thulium	<0.008
Cadmium	<0.008	Iodine	≤0.005	Praseodymium	<0.008	Tin	<0.008
Calcium	MC	Iridium	<0.008	Rhenium	<0.008	Titanium	0.3 ± .25
Cerium	0.007 ± .002	Iron	3.5 ± .5	Rhodium	<0.008	Tungsten	<0.008
Cesium	≤0.005	Lanthanum	0.005 ± 0	Rubidium	0.15 ± .05	Uranium	<0.008
Chlorine	2	Lead	≤0.04	Ruthenium	0.008	Vandium	0.003 ± .001
Chromium	0.025 ± .005	Lithium	0.7 ± .3	Samarium	<0.008	Ytterbium	<0.008
Cobalt	0.009 ± .001	Lutetium	<0.008	Scandium	≤0.01	Yttrium	<0.008
Copper	0.08 ± .02	Magnesium	MC	Selenium	0.008 ± .002	Zinc	0.1 ± 0
Dysprosium	<0.008	Manganese	0.3 ± .1	Silicon	5 ± 2	Zirconium	0.01 ± 0
Erbium	<0.008	Mercury[b]	<0.009	Silver	<0.008		
Europium	<0.008	Molybdenum	0.025 ± .005	Sodium	MC		

---

[a] Detection limit was 0.008.

[b] Determined by flameless atomic absorption.

Table B25. ELEMENTAL CONCENTRATIONS IN WATER SAMPLE (-17L) FROM WELL DW-5 FROM IN SITU COAL GASIFICATION EXPERIMENT (LLL)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	0.17 ± .13	Fluorine	≃6	Neodymium	<0.008	Strontium	6 ± 0
Antimony	<0.008	Gadolinium	<0.008	Nickel	0.06 ± 0	Sulfur	MC
Arsenic	0.009 ± .001	Gallium	0.008 ± .002	Niobium	<0.008	Tantalum	<0.008
Barium	0.08 ± .02	Germanium	<0.008	Osmium	<0.008	Tellurium	<0.008
Beryllium	<0.008	Gold	<0.008	Palladium	<0.008	Terbium	<0.008
Bismuth	<0.008	Hafnium	<0.008	Phosphorus	0.3 ± .1	Thallium	<0.008
Boron	0.15 ± .05	Holmium	<0.008	Platinum	<0.008	Thorium	<0.008
Bromine	0.04 ± .02	Indium	[illegible]	Potassium	MC	Thulium	<0.008
Cadmium	<0.008	Iodine	0.008 ± 0	Praseodymium	<0.008	Tin	<0.008
Calcium	MC	Iridium	<0.008	Rhenium	<0.008	Titanium	0.15 ± .05
Cerium	0.008 ± .002	Iron	7 ± 3	Rhodium	<0.008	Tungsten	<0.008
Cesium	0.005 ± .002	Lanthanum	<0.008	Rubidium	0.15 ± .05	Uranium	<0.008
Chlorine	4.5 ± 2.5	Lead	0.06 ± .01	Ruthenium	<0.008	Vandium	0.003 ± 0
Chromium	0.02 ± 0	Lithium	0.7 ± .3	Samarium	<0.008	Ytterbium	<0.008
Cobalt	0.03 ± .01	Lutetium	<0.008	Scandium	0.02 ± .01	Yttrium	0.006 ± 0
Copper	0.06 ± .02	Magnesium	MC	Selenium	0.015 ± .005	Zinc	0.2 ± 0
Dysprosium	<0.008	Manganese	0.6 ± .1	Silicon	4 ± 2	Zirconium	0.01 ± 0
Erbium	<0.008	Mercury[b]	<0.009	Silver	<0.008		
Europium	<0.008	Molybdenum	0.04 ± .01	Sodium	MC		

[a] Detection limit was 0.008.

[b] Determined by flameless atomic absorption.

Table B26. ELEMENTAL CONCENTRATIONS IN WATER SAMPLE (-18L) FROM WELL DW-4 FROM *IN SITU* COAL GASIFICATION EXPERIMENT (LLL)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	0.05 ± .05	Fluorine	≈4	Neodymium	<0.005	Strontium	0.3 ± .2
Antimony	<0.005	Gadolinium	<0.005	Nickel	0.04 ± .01	Sulfur	MC
Arsenic	0.005 ± .004	Gallium	0.007 ± .002	Niobium	<0.005	Tantalum	<0.005
Barium	0.025 ± .005	Germanium	<0.005	Osmium	<0.005	Tellurium	<0.005
Beryllium	<0.005	Gold	<0.005	Palladium	<0.005	Terbium	<0.005
Bismuth	<0.005	Hafnium	<0.005	Phosphorus	0.13 ± .07	Thallium	<0.005
Boron	0.14 ± .06	Holmium	<0.005	Platinum	<0.005	Thorium	<0.005
Bromine	0.35 ± .05	Indium	[illegible]	Potassium	<0.005	Thulium	<0.005
Cadmium	<0.005	Iodine	0.007 ± .007	Praseodymium	<0.005	Tin	<0.005
Calcium	8 ± 6	Iridium	<0.005	Rhenium	<0.005	Titanium	0.09 ± .01
Cerium	<0.005	Iron	3 ± 0	Rhodium	<0.005	Tungsten	<0.005
Cesium	0.006 ± .001	Lanthanum	<0.005	Rubidium	0.16 ± .14	Uranium	<0.005
Chlorine	4 ± 0	Lead	≤0.05	Ruthenium	<0.005	Vandium	0.005 ± .001
Chromium	0.006 ± .001	Lithium	0.3 ± 0	Samarium	<0.005	Ytterbium	<0.005
Cobalt	0.004 ± .002	Lutetium	<0.005	Scandium	0.015 ± .005	Yttrium	<0.005
Copper	0.3 ± 0	Magnesium	2.5 ± 1.5	Selenium	0.014 ± .006	Zinc	0.05 ± .02
Dysprosium	<0.005	Manganese	0.01 ± 0	Silicon	2.2 ± 1.8	Zirconium	0.007 ± .003
Erbium	<0.005	Mercury[b]	<0.009	Silver	<0.005		
Europium	<0.005	Molybdenum	0.06 ± .03	Sodium	MC		

---

[a] Detection limit was 0.005.

[b] Determined by flamless atomic absorption.

Table B27. ELEMENTAL CONCENTRATIONS IN WATER SAMPLE (-19L) FROM PRODUCTION WELL #1 AFTER IN SITU COAL GASIFICATION (LLL)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	0.07 ± .04	Fluorine	≈3	Neodymium	<0.01	Strontium	7 ± 2
Antimony	<0.01	Gadolinium	<0.01	Nickel	0.025 ± .005	Sulfur	MC
Arsenic	0.01 ± 0	Gallium	0.015 ± .005	Niobium	<0.01	Tantalum	<0.01
Barium	0.055 ± .005	Germanium	<0.01	Osmium	<0.01	Tellurium	<0.01
Beryllium	<0.01	Gold	<0.01	Palladium	<0.01	Terbium	<0.01
Bismuth	<0.01	Hafnium	<0.01	Phosphorus	0.5 ± .2	Thallium	<0.01
Boron	0.05 ± 0	Holmium	<0.01	Platinum	<0.01	Thorium	<0.01
Bromine	0.01 ± .01	Indium	[illegible]	Potassium	MC	Thulium	<0.01
Cadmium	<0.01	Iodine	0.01 ± 0	Praseodymium	<0.01	Tin	<0.01
Calcium	MC	Iridium	<0.01	Rhenium	<0.01	Titanium	0.1 ± 0
Cerium	<0.01	Iron	0.9 ± .1	Rhodium	<0.01	Tungsten	<0.01
Cesium	0.009 ± .001	Lanthanum	<0.01	Rubidium	0.08 ± .02	Uranium	<0.01
Chlorine	2 ± 0	Lead	0.07 ± .01	Ruthenium	<0.01	Vandium	0.004 ± .001
Chromium	0.03 ± .01	Lithium	0.7 ± .3	Samarium	<0.01	Ytterbium	<0.01
Cobalt	0.015 ± .005	Lutetium	<0.01	Sandium	0.03 ± .01	Yttrium	<0.01
Copper	0.18 ± .12	Magnesium	MC	Selenium	<0.01	Zinc	0.08 ± .02
Dysprosium	<0.01	Manganese	0.3 ± .1	Silicon	MC	Zirconium	0.015 ± .005
Erbium	<0.01	Mercury[b]	<0.009	Silver	<0.01		
Europium	<0.01	Molybdenum	0.07 ± .03	Sodium	MC		

[a] Detection limit was 0.01.

[b] Determined by flameless atomic absorption.

Table B28. ELEMENTAL CONCENTRATIONS IN WATER SAMPLE (-20L) FROM PRODUCTION WELL #1 AFTER IN SITU COAL GASIFICATION (LLL)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	0.3 ± 0	Fluorine	≈5	Neodymium	<0.009	Strontium	MC
Antimony	<0.009	Gadolinium	<0.009	Nickel	0.07 ± .04	Sulfur	MC
Arsenic	0.025 ± .005	Gallium	0.05 ± .03	Niobium	<0.009	Tantalum	<0.009
Barium	0.09 ± .01	Germanium	0.015 ± .005	Osmium	<0.009	Tellurium	<0.009
Beryllium	<0.009	Gold	<0.009	Palladium	<0.009	Terbium	<0.009
Bismuth	<0.009	Hafnium	<0.009	Phosphorus	1.4 ± 0.6	Thallium	<0.009
Boron	0.5 ± .1	Holmium	<0.009	Platinum	<0.009	Thorium	<0.009
Bromine	0.15 ± .05	Indium	[illegible]	Potassium	MC	Thulium	<0.009
Cadmium	<0.009	Iodine	0.02 ± 0	Praseodymium	<0.009	Tin	<0.009
Calcium	MC	Iridium	<0.009	Rhenium	<0.009	Titanium	0.15 ± .05
Cerium	0.008 ± .002	Iron	4 ± 1	Rhodium	<0.009	Tungsten	<0.009
Cesium	0.008 ± .001	Lanthanum	<0.009	Rubidium	0.2 ± 0	Uranium	<0.009
Chlorine	3 ± 0	Lead	0.12 ± .08	Ruthenium	<0.009	Vandium	0.007 ± .001
Chromium	0.06 ± .01	Lithium	0.6 ± .4	Samarium	<0.009	Ytterbium	<0.009
Cobalt	0.013 ± .006	Lutetium	<0.009	Sandium	0.025 ± .005	Yttrium	0.005 ± .001
Copper	0.3 ± .1	Magnesium	MC	Selenium	0.02 ± 0	Zinc	0.15 ± .05
Dysprosium	<0.009	Manganese	0.055 ± .005	Silicon	2.2 ± 1.9	Zirconium	0.014 ± .006
Erbium	<0.009	Mercury[b]	<0.009	Silver	<0.009		
Europium	<0.009	Molybdenum	<0.009	Sodium	MC		

[a] Detection limit was 0.009.

[b] Determined by flameless atomic absorption.

Table B29. ELEMENTAL CONCENTRATIONS IN SEAM WATER FROM WELL #6 (HANNA #2) PRIOR TO IN SITU COAL GASIFICATION (LERC)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	0.11 ± .09	Fluorine	≈2 ± 0	Neodymium	0.002 ± .001	Strontium	0.24 ± .36
Antimony	<0.001	Gadolinium	0.001 ± .001	Nickel	0.07 ± .004	Sulfur	5
Arsenic	0.010 ± .009	Gallium	0.004 ± .002	Niobium	0.001 ± .001	Tantalum	<0.001
Barium	0.05 ± .03	Germanium	0.005 ± .003	Osmium	<0.001	Tellurium	<0.001
Beryllium	<0.001	Gold	<0.001	Palladium	<0.001	Terbium	<0.001
Bismuth	<0.001	Hafnium	<0.001	Phosphorus	0.1 ± 0.1	Thallium	<0.001
Boron	0.02 ± 0	Holmium	<0.001	Platinum	<0.001	Thorium	<0.001
Bromine	0.015 ± .005	Indium	[illegible]	Potassium	MC	Thulium	<0.001
Cadmium	<0.001	Iodine	.001 ± .001	Praseodymium	0.001 ± .001	Tin	0.006 ± .002
Calcium	MC	Iridium	<0.001	Rhenium	<0.001	Titanium	0.5 ± .4
Cerium	<0.001	Iron	MC	Rhodium	<0.001	Tungsten	<0.001
Cesium	0.001 ± .001	Lanthanum	<0.001	Rubidium	0.06 ± .06	Uranium	0.001 ± .001
Chlorine	4 ± 2	Lead	0.02 ± .1	Ruthenium	<0.001	Vandium	0.003 ± .001
Chromium	0.009 ± .001	Lithium	0.5 ± .5	Samarium	0.001 ± .001	Ytterbium	<0.001
Cobalt	0.007 ± .002	Lutetium	<0.001	Scandium	0.006 ± .002	Yttrium	<0.001
Copper	0.19 ± .09	Magnesium	MC	Selenium	0.008 ± .002	Zinc	0.35 ± .05
Dysprosium	<0.001	Manganese	0.5 ± .1	Silicon	MC	Zirconium	0.004 ± .003
Erbium	<0.001	Mercury[b]	<0.0004	Silver	0.001 ± .001		
Europium	<0.001	Molybdenum	0.3 ± .033	Sodium	MC		

---

[a] Detection limit was 0.001

[b] Detected by flameless atomic absorption.

Table B30. ELEMENTAL CONCENTRATIONS IN SEAM WATER FROM WELL #5 (HANNA #2) PRIOR TO IN SITU COAL GASIFICATION (LERC)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	0.7 ± .4	Fluorine	≈0.6	Neodymium	0.001 ± .001	Strontium	0.06 ± .01
Antimony	0.001 ± .001	Gadolinium	<0.001	Nickel	0.04 ± .03	Sulfur	MC
Arsenic	0.004 ± .001	Gallium	0.005 ± .004	Niobium	<0.001	Tantalum	<0.001
Barium	0.013 ± .007	Germanium	0.001 ± 0	Osmium	<0.001	Tellurium	<0.001
Beryllium	<0.001	Gold	<0.001	Palladium	<0.001	Terbium	<0.001
Bismuth	<0.001	Hafnium	<0.001	Phosphorus	0.08 ± .02	Thallium	<0.001
Boron	0.003 ± .001	Holmium	<0.001	Platinum	<0.001	Thorium	<0.001
Bromine	0.02 ± .01	Indium	[illegible]	Potassium	MC	Thulium	<0.001
Cadmium	<0.001	Iodine	0.001 ± .001	Praseodymium	<0.001	Tin	<0.001
Calcium	MC	Iridium	<0.001	Rhenium	<0.001	Titanium	0.12 ± .08
Cerium	0.001	Iron	MC	Rhodium	<0.001	Tungsten	<0.001
Cesium	0.001 ± .001	Lanthanum	0.001 ± 0	Rubidium	0.005 ± .02	Uranium	<0.001
Chlorine	2 ± 0	Lead	0.009 ± .01	Ruthenium	<0.001	Vandium	0.005 ± .002
Chromium	0.009 ± .001	Lithium	0.5 ± .5	Samarium	0.001 ± .001	Ytterbium	<0.001
Cobalt	0.008 ± .002	Lutetium	<0.001	Scandium	0.007 ± .001	Yttrium	<0.001
Copper	0.25 ± .15	Magnesium	~2	Selenium	0.004 ± .001	Zinc	0.2 ± .09
Dysprosium	<0.001	Manganese	0.19 ± .11	Silicon	2	Zirconium	0.005 ± .001
Erbium	<0.001	Mercury[b]	0.0011	Silver	0.001 ± .001		
Europium	<0.001	Molybdenum	0.05 ± .02	Sodium	MC		

[a] Detection limit was 0.001.

[b] Detected by flameless atomic absorption.

Table B31. ELEMENTAL CONCENTRATIONS IN PRODUCT WATER (-8L) FROM WELL 5-6 LINKAGE DURING IN SITU COAL GASIFICATION (LERC)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	7.5 ± 2.5	Fluorine	1.4 ± .6	Neodymium	<0.2	Strontium	0.2 ± 0
Antimony	<0.2	Gadolinium	<0.2	Nickel	0.35 ± .05	Sulfur	10.5 ± 1.5
Arsenic	<0.1	Gallium	0.1 ± 0	Niobium	<0.2	Tantalum	<0.2
Barium	0.25 ± .05	Germanium	<0.2	Osmium	<0.2	Tellurium	<0.2
Beryllium	<0.1	Gold	<0.2	Palladium	<0.2	Terbium	<0.2
Bismuth	<0.2	Hafnium	<0.2	Phosphorus	5 ± 2	Thallium	<0.2
Boron	<0.1	Holmium	<0.2	Platinum	<0.2	Thorium	<0.2
Bromine	<0.1	Indium	[illegible]	Potassium	4.5 ± 1.5	Thulium	<0.2
Cadmium	<0.2	Iodine	<0.2	Praseodymium	<0.2	Tin	<0.2
Calcium	24 ± 6	Iridium	<0.2	Rhenium	<0.2	Titanium	3 ± 1
Cerium	<0.2	Iron	4.5 ± 1.5	Rhodium	<0.2	Tungsten	<0.2
Cesium	0.05 ± .05	Lanthanum	<0.2	Rubidium	0.1 ± 1	Uranium	<0.2
Chlorine	0.75 ± .25	Lead	0.55 ± .15	Ruthenium	<0.2	Vandium	<0.1
Chromium	0.45 ± .15	Lithium	0.1 ± 0	Samarium	<0.2	Ytterbium	<0.2
Cobalt	<0.1	Lutetium	<0.2	Scandium	0.3 ± .1	Yttrium	<0.1
Copper	0.75 ± .05	Magnesium	9 ± 1	Selenium	<0.1	Zinc	0.6 ± .2
Dysprosium	<0.2	Manganese	0.2 ± .1	Silicon	18 ± 10	Zirconium	<0.1
Erbium	<0.2	Mercury[b]	0.002	Silver	<0.2		
Europium	<0.2	Molybdenum	0.5 ± 0	Sodium	17 ± 1		

---

[a] Detection limit was 0.1.

[b] Determined by flameless atomic absorption.

Table B32. ELEMENTAL CONCENTRATIONS IN PRODUCT WATER (-9L) FROM WELL 5-6 LINKAGE DURING IN SITU COAL GASIFICATION (LERC)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	1.6 ± 1.4	Fluorine	<.001	Neodymium	<.001	Strontium	0.017 ± .012
Antimony	0.01 ± 0	Gadolinium	<.001	Nickel	0.355 ± .345	Sulfur	≥8
Arsenic	0.045 ± .043	Gallium	0.004 ± .002	Niobium	<.001	Tantalum	<.001
Barium	0.2 ± 1	Germanium	0.055 ± .015	Osmium	<.001	Tellurium	<.001
Beryllium	<.001	Gold	<.001	Palladium	<.001	Terbium	<.001
Bismuth	0.002 ± .002	Hafnium	<.001	Phosphorus	0.25 ± .15	Thallium	<.001
Boron	0.0245 ± .015	Holmium	<.001	Platinum	<.001	Thorium	0.002 ± .001
Bromine	<.001	Indium	[illegible]	Potassium	0.55 ± .35	Thulium	<.001
Cadmium	0.025 ± .005	Iodine	0.001 ± .001	Praseodymium	0.001 ± .001	Tin	0.6 ± .2
Calcium	2 ± 1	Iridium	<.001	Rhenium	<.001	Titanium	0.12 ± .08
Cerium	0.003 ± .002	Iron	2.5 ± .5	Rhodium	<.001	Tungsten	≤0.004 ± .001
Cesium	0.001 ± .001	Lanthanum	0.002 ± .002	Rubidium	0.003 ± .001	Uranium	0.002 ± 0
Chlorine	0.115 ± .085	Lead	0.008 ± .002	Ruthenium	<.001	Vandium	0.003 ± .002
Chromium	0.03 ± .02	Lithium	0.023 ± .016	Samarium	<.001	Ytterbium	<.001
Cobalt	0.003 ± .001	Lutetium	<.001	Scandium	0.002 ± .001	Yttrium	<.001
Copper	0.395 ± .30	Magnesium	MC	Selenium	0.03 ± 0	Zinc	0.02 ± .01
Dysprosium	<.001	Manganese	0.0125 ± .007	Silicon	3	Zirconium	0.01 ± .01
Erbium	<.001	Mercury[b]	0.0018	Silver	<.001		
Europium	<.001	Molybdenum	0.01 ± .001	Sodium	<.001		

---

[a] Detection limit was 0.001.

[b] Determined by flameless atomic absorption.

Table B33. ELEMENTAL CONCENTRATIONS IN PRODUCT TAR (-10S) FROM WELL 5-6 LINKAGE DURING IN SITU COAL GASIFICATION (LERC)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	1.5 ± .5	Fluorine	0.03 ± .01	Neodymium	<.002	Strontium	0.01 ± 0
Antimony	0.012 ± .010	Gadolinium	<.002	Nickel	0.4 ± .1	Sulfur	1.4 ± .6
Arsenic	0.8 ± .2	Gallium	0.015 ± .005	Niobium	<.002	Tantalum	<.002
Barium	0.09 ± .01	Germanium	0.06 ± .02	Osmium	<.002	Tellurium	<.002
Beryllium	<.002	Gold	<.002	Palladium	<.002	Terbium	<.002
Bismuth	0.006 ± .003	Hafnium	<.002	Phosphorus	1.75 ± 1.25	Thallium	<.002
Boron	0.04 ± .01	Holmium	<.002	Platinum	<.002	Thorium	0.002 ± .002
Bromine	0.003 ± .003	Indium	[illegible]	Potassium	0.25 ± .05	Thulium	<.002
Cadmium	0.09 ± .01	Iodine	0.002 ± .002	Praseodymium	<.002	Tin	3 ± 0
Calcium	5	Iridium	<.002	Rhenium	<.002	Titanium	0.2 ± 0
Cerium	0.002 ± .001	Iron	6 ± 2	Rhodium	<.002	Tungsten	≤0.006 ± .006
Cesium	0.002 ± .001	Lanthanum	0.001 ± .001	Rubidium	0.004 ± .001	Uranium	0.002 ± .002
Chlorine	0.1 ± 1	Lead	0.06 ± .03	Ruthenium	<.002	Vandium	0.007 ± .003
Chromium	0.12 ± .08	Lithium	0.02 ± .01	Samarium	<.002	Ytterbium	<.002
Cobalt	0.008 ± .002	Lutetium	<.002	Scandium	0.001 ± .001	Yttrium	0.001 ± .001
Copper	0.7 ± .2	Magnesium	2.5 ± 1.5	Selenium	0.03 ± .03	Zinc	0.45 ± .05
Dysprosium	<.002	Manganese	0.13 ± .07	Silicon	MC	Zirconium	0.004 ± .001
Erbium	<.002	Mercury[b]	<0.23	Silver	.002		
Europium	<.002	Molybdenum	0.03 ± .01	Sodium	≳6		

[a] Detection limit was 0.002.

[b] Determined by flameless atomic absorption.

Table B34. ELEMENTAL CONCENTRATIONS IN PRODUCT WATER (-11L) FROM WELL 5-6 LINKAGE DURING IN SITU COAL GASIFICATION (LERC)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	2 ± 1	Fluorine	0.055 ± .005	Neodymium	<.002	Strontium	0.03 ± .02
Antimony	0.003 ± .001	Gadolinium	<.002	Nickel	0.03 ± .01	Sulfur	2
Arsenic	0.05 ± 0	Gallium	0.026 ± .23	Niobium	<.002	Tantalum	<.002
Barium	0.045 ± .015	Germanium	0.14 ± .06	Osmium	<.002	Tellurium	<.002
Beryllium	<.002	Gold	<.002	Palladium	<.002	Terbium	<.002
Bismuth	0.004 ± .002	Hafnium	<.002	Phosphorus	0.07 ± .01	Thallium	<.002
Boron	0.04 ± .01	Holmium	<.002	Platinum	<.002	Thorium	0.002 ± .001
Bromine	0.003 ± 0	Indium	[illegible]	Potassium	2.6 ± 2.4	Thulium	<.002
Cadmium	0.01 ± .01	Iodine	0.002 ± 0	Praseodymium	<.002	Tin	0.09 ± .01
Calcium	3.5 ± .5	Iridium	<.002	Rhenium	<.002	Titanium	0.15 ± .05
Cerium	0.001 ± .001	Iron	0.45 ± .05	Rhodium	<.002	Tungsten	0.008 ± 0
Cesium	0.001 ± .001	Lanthanum	0.003 ± .003	Rubidium	0.004 ± .001	Uranium	0.003 ± .001
Chlorine	0.145 ± .055	Lead	0.03 ± .02	Ruthenium	<.002	Vandium	0.005 ± .001
Chromium	0.06 ± .03	Lithium	0.052 ± .048	Samarium	<.002	Ytterbium	<.002
Cobalt	0.004 ± .001	Lutetium	<.002	Scandium	0.003 ± .001	Yttrium	0.001 ± .001
Copper	0.1 ± 0	Magnesium	2 ± 1	Selenium	0.05 ± .01	Zinc	0.015 ± .005
Dysprosium	<.002	Manganese	0.009 ± .001	Silicon	6 ± 1	Zirconium	0.006 ± .001
Erbium	<.002	Mercury[b]	0.0260	Silver	0.003 ± .003		
Europium	<.002	Molybdenum	0.21 ± .19	Sodium	MC		

[a] Detection limit was 0.002.

[b] Determined by flameless atomic absorption.

Table B35. ELEMENTAL CONCENTRATIONS IN PRODUCT TAR (-12S) FROM WELL 5-6 DURING IN SITU COAL GASIFICATION (LERC)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	MC	Fluorine	4 ± 0	Neodymium	0.008 ± .008	Strontium	0.2 ± .1
Antimony	0.02 ± .01	Gadolinium	<.002	Nickel	0.1 ± 0	Sulfur	MC
Arsenic	0.8 ± .1	Gallium	0.15 ± .05	Niobium	0.002 ± .002	Tantalum	<.002
Barium	0.55 ± .05	Germanium	0.3 ± 0	Osmium	<.002	Tellurium	0.005 ± .005
Beryllium	0.001 ± 0	Gold	<.002	Palladium	<.002	Terbium	<.002
Bismuth	0.055 ± .025	Hafnium	<.002	Phosphorus	1.5 ± .5	Thallium	<.002
Boron	0.05 ± .02	Holmium	<.002	Platinum	<.002	Thorium	0.002 ± .001
Bromine	0.002 ± .002	Indium	[illegible]	Potassium	MC	Thulium	<.002
Cadmium	0.5 ± .1	Iodine	0.001 ± .001	Praseodymium	0.002 ± 0	Tin	0.45 ± .15
Calcium	MC	Iridium	<.002	Rhenium	<.002	Titanium	6 ± 2
Cerium	0.025 ± .005	Iron	MC	Rhodium	<.002	Tungsten	0.006 ± .002
Cesium	0.003 ± .001	Lanthanum	0.014 ± .006	Rubidium	0.13 ± .06	Uranium	0.002 ± .001
Chlorine	0.4 ± .1	Lead	2.5 ± .5	Ruthenium	<.002	Vandium	0.08 ± .01
Chromium	0.3 ± .1	Lithium	0.09 ± .01	Samarium	0.006 ± .006	Ytterbium	<.002
Cobalt	0.04 ± 0	Lutetium	<.002	Scandium	0.02 ± .01	Yttrium	0.008 ± .002
Copper	1.8 ± 1.1	Magnesium	MC	Selenium	0.08 ± .01	Zinc	3 ± 2
Dysprosium	<.002	Manganese	0.5 ± .2	Silicon	MC	Zirconium	0.035 ± .005
Erbium	<.002	Mercury[b]	<0.23	Silver	0.03 ± .03		
Europium	0.002 ± .002	Molybdenum	0.054 ± .046	Sodium	MC		

---

[a] Detection limit was 0.002

[b] Determined by flameless atomic absorption.

Table B36. ELEMENTAL CONCENTRATIONS IN PRODUCT WATER (-13L) FROM WELL 5-6 LINKAGE DURING *IN SITU* COAL GASIFICATION (LERC)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	0.15 ± 0.5	Fluorine	0.035 ± .005	Neodymium	<.005	Strontium	0.014 ± .006
Antimony	0.005 ± .003	Gadolinium	<.005	Nickel	0.05 ± .01	Sulfur	3.5 ± .5
Arsenic	0.03 ± .02	Gallium	0.003 ± .001	Niobium	<.005	Tantalum	<.005
Barium	0.15 ± .05	Germanium	0.07 ± .01	Osmium	<.005	Tellurium	<.005
Beryllium	<.005	Gold	<.005	Palladium	<.005	Terbium	<.005
Bismuth	0.003 ± .001	Hafnium	<.005	Phosphorus	0.06 ± .01	Thallium	<.005
Boron	0.014 ± .006	Holmium	<.005	Platinum	<.005	Thorium	0.004 ± .002
Bromine	0.003 ± .001	Indium	[illegible]	Potassium	0.2 ± .1	Thulium	<.005
Cadmium	<.005	Iodine	0.002 ± .001	Praseodymium	<.005	Tin	0.04 ± .01
Calcium	2.5 ± .5	Iridium	<.005	Rhenium	<.005	Titanium	0.04 ± .02
Cerium	0.003 ± .001	Iron	0.5 ± .2	Rhodium	<.005	Tungsten	0.007 ± .002
Cesium	0.002 ± .001	Lanthanum	0.002 ± .001	Rubidium	0.002 ± .001	Uranium	0.004 ± .002
Chlorine	0.2 ± .1	Lead	0.03 ± .01	Ruthenium	<.005	Vandium	0.001 ± .001
Chromium	0.02 ± 0	Lithium	0.02 ± .01	Samarium	<.005	Ytterbium	<.005
Cobalt	0.001 ± 0	Lutetium	<.005	Scandium	0.002 ± 0	Yttrium	0.001 ± .001
Copper	0.25 ± .05	Magnesium	1.8 ± 1.1	Selenium	0.02 ± 0	Zinc	0.06 ± .05
Dysprosium	<.005	Manganese	0.004 ± .001	Silicon	6	Zirconium	0.004 ± .002
Erbium	<.005	Mercury[b]	0.0215	Silver	0.002 ± .002		
Europium	<.005	Molybdenum	0.07 ± .02	Sodium	MC		

[a] Detection limit was 0.005.

[b] Determined by flameless atomic absorption.

Table B37. ELEMENTAL CONCENTRATIONS IN PRODUCT WATER (-14L) FROM WELL 7-8 *IN SITU* COAL GASIFICATION (LERC)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	0.08 ± .02	Fluorine	0.16 ± .16	Neodymium	<.005	Strontium	0.015 ± .005
Antimony	<.005	Gadolinium	<.005	Nickel	0.1 ± 0	Sulfur	6.5 ± 3.5
Arsenic	0.025 ± .005	Gallium	<.005	Niobium	<.005	Tantalum	<.005
Barium	0.14 ± .09	Germanium	0.02 ± 0	Osmium	<.005	Tellurium	<.005
Beryllium	<.005	Gold	<.005	Palladium	<.005	Terbium	<.005
Bismuth	<.005	Hafnium	<.005	Phosphorus	0.8 ± .2	Thallium	<.005
Boron	0.15 ± .05	Holmium	<.005	Platinum	<.005	Thorium	<.005
Bromine	<.005	Indium	[illegible]	Potassium	0.5 ± .2	Thulium	<.005
Cadmium	<.005	Iodine	<.005	Praseodymium	<.005	Tin	0.08 ± .01
Calcium	7 ± 1	Iridium	<.005	Rhenium	<.005	Titanium	0.07 ± .02
Cerium	<.005	Iron	0.55 ± .05	Rhodium	<.005	Tungsten	<.005
Cesium	<.005	Lanthanum	<.005	Rubidium	0.006 ± .001	Uranium	<.005
Chlorine	0.425 ± .375	Lead	0.04 ± 0	Ruthenium	<.005	Vandium	0.001 ± 0
Chromium	0.075 ± .025	Lithium	0.001 ± 0	Samarium	<.005	Ytterbium	<.005
Cobalt	0.005 ± 0	Lutetium	<.005	Scandium	0.002 ± 0	Yttrium	<.005
Copper	0.15 ± .05	Magnesium	5.2 ± 3.0	Selenium	<.005	Zinc	0.06 ± .02
Dysprosium	<.005	Manganese	0.02 ± 0	Silicon	7.5 ± .5	Zirconium	<.005
Erbium	<.005	Mercury[b]	0.0300	Silver	0.1 ± .1		
Europium	<.005	Molybdenum	0.02 ± .02	Sodium	MC		

[a] Detection limit was 0.005.

[b] Determined by flameless atomic absorption.

Table B38. ELEMENTAL CONCENTRATIONS IN PRODUCT TAR (-15S) FROM WELL 7-8 IN SITU COAL GASIFICATION (LERC)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	0.25 ± .05	Fluorine	0.4 ± .2	Neodymium	<.01	Strontium	0.019 ± .011
Antimony	<.01	Gadolinium	<.01	Nickel	0.3 ± 0	Sulfur	6 ± 4
Arsenic	0.25 ± .04	Gallium	0.01 ± .01	Niobium	<.01	Tantalum	<.01
Barium	0.055 ± .005	Germanium	0.08 ± .02	Osmium	<.01	Tellurium	<.01
Beryllium	<.01	Gold	<.01	Palladium	<.01	Terbium	<.01
Bismuth	0.05 ± .05	Hafnium	<.01	Phosphorus	0.9 ± 0	Thallium	<.01
Boron	0.6 ± .3	Holmium	<.01	Platinum	<.01	Thorium	<.01
Bromine	<.01	Indium	[illegible]	Potassium	0.5 ± .3	Thulium	<.01
Cadmium	≤0.2 ± .2	Iodine	<.01	Praseodymium	<.01	Tin	0.1 ± .1
Calcium	8 ± 1	Iridium	<.01	Rhenium	<.01	Titanium	0.5 ± .3
Cerium	<.01	Iron	5.5 ± 1.5	Rhodium	<.01	Tungsten	<.01
Cesium	<.01	Lanthanum	<.01	Rubidium	0.03 ± .03	Uranium	<.01
Chlorine	1.6 ± 1.4	Lead	0.135 ± .065	Ruthenium	<.01	Vandium	0.01 ± 0
Chromium	0.6 ± .1	Lithium	0.003 ± .001	Samarium	<.01	Ytterbium	<.01
Cobalt	0.015 ± .005	Lutetium	<.01	Scandium	0.004 ± .001	Yttrium	<.01
Copper	4 ± 1	Magnesium	3.8 ± 3.2	Selenium	<.01	Zinc	1.8 ± 1.2
Dysprosium	<.01	Manganese	0.135 ± .065	Silicon	MC	Zirconium	<.01
Erbium	<.01	Mercury[b]	<0.23	Silver	<.01		
Europium	<.01	Molybdenum	0.04 ± .01	Sodium	8 ± 2		

[a] Detection limit was .01.

[b] Determined by flameless atomic absorption.

Table B39. ELEMENTAL CONCENTRATIONS IN PRODUCT WATER (-16L) FROM WELL 7-8 IN SITU COAL GASIFICATION (LERC)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	0.185 ± .115	Fluorine	0.04 ± .02	Neodymium	<.005	Strontium	0.015 ± .005
Antimony	<.005	Gadolinium	<.005	Nickel	0.08 ± .02	Sulfur	4.5 ± .5
Arsenic	0.04 ± .03	Gallium	<.005	Niobium	<.005	Tantalum	<.005
Barium	0.0075 ± .0025	Germanium	0.05 ± .03	Osmium	<.005	Tellurium	<.005
Beryllium	<.005	Gold	<.005	Palladium	<.005	Terbium	<.005
Bismuth	<.005	Hafnium	<.005	Phosphorus	0.145 ± .055	Thallium	<.005
Boron	0.4 ± .2	Holmium	<.005	Platinum	<.005	Thorium	<.005
Bromine	<.005	Indium	[illegible]	Potassium	0.35 ± .25	Thulium	<.005
Cadmium	<.005	Iodine	<.005	Praseodymium	<.005	Tin	0.05 ± 0
Calcium	8 ± 2	Iridium	<.005	Rhenium	<.005	Titanium	0.07 ± .01
Cerium	<.005	Iron	1.8 ± 1.6	Rhodium	<.005	Tungsten	<.005
Cesium	<.005	Lanthanum	<.005	Rubidium	<.005	Uranium	<.005
Chlorine	0.15 ± .05	Lead	0.03 ± .01	Ruthenium	<.005	Vandium	<.005
Chromium	0.3 ± .1	Lithium	0.002 ± .001	Samarium	<.005	Ytterbium	<.005
Cobalt	0.003 ± 0	Lutetium	<.005	Scandium	0.003 ± .001	Yttrium	<.005
Copper	0.3 ± 0	Magnesium	1.5 ± .5	Selenium	<.005	Zinc	.055 ± .015
Dysprosium	<.005	Manganese	0.07 ± .01	Silicon	5 ± 2	Zirconium	<.005
Erbium	<.005	Mercury[b]	0.0020	Silver	<.005		
Europium	<.005	Molybdenum	0.02 ± .01	Sodium	MC		

[a] Detection limit was 0.005.

[b] Determined by flameless atomic absorption.

Table B40. ELEMENTAL CONCENTRATIONS IN PRODUCT TAR (-17S) FROM WELL 7-8 IN SITU COAL GASIFICATION (LERC)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	0.25 ± .05	Fluorine	0.11 ± .09	Neodymium	<.01	Strontium	0.006 ± .002
Antimony	<.01	Gadolinium	<.01	Nickel	0.15 ± .05	Sulfur	0.4 ± .1
Arsenic	0.25 ± .05	Gallium	<.01	Niobium	<.01	Tantalum	<.01
Barium	0.02 ± 0	Germanium	0.035 ± .005	Osmium	<.01	Tellurium	<.01
Beryllium	<.01	Gold	<.01	Palladium	<.01	Terbium	<.01
Bismuth	<.01	Hafnium	<.01	Phosphorus	0.2 ± 0	Thallium	<.01
Boron	0.04 ± .02	Holmium	<.01	Platinum	<.01	Thorium	<.01
Bromine	<.01	Indium	[illegible]	Potassium	0.2 ± 0	Thulium	<.01
Cadmium	<.01	Iodine	<.01	Praseodymium	<.01	Tin	0.05 ± .01
Calcium	4.5 ± 2.5	Iridium	<.01	Rhenium	<.01	Titanium	0.09 ± .01
Cerium	<.01	Iron	3 ± 1.5	Rhodium	<.01	Tungsten	<.01
Cesium	<.01	Lanthanum	<.01	Rubidium	<.01	Uranium	<.01
Chlorine	0.4 ± .2	Lead	0.09 ± .01	Ruthenium	<.01	Vandium	0.002 ± .002
Chromium	0.6 ± .2	Lithium	0.022 ± .020	Samarium	<.01	Ytterbium	<.01
Cobalt	0.007 ± .006	Lutetium	<.01	Scandium	0.003 ± .001	Yttrium	<.01
Copper	0.75 ± .05	Magnesium	0.45 ± .05	Selenium	<.01	Zinc	0.3 ± .1
Dysprosium	<.01	Manganese	0.05 ± .01	Silicon	5 ± 1	Zirconium	<.01
Erbium	<.01	Mercury[b]	<0.23	Silver	<.01		
Europium	<.01	Molybdenum	0.03 ± 0	Sodium	3 ± 2.9		

[a] Detection limit was 0.01.

[b] Detected by flameless atomic absorption.

Table B41. ELEMENTAL CONCENTRATIONS IN PRODUCT WATER (-18L) FROM WELL 7-8 IN SITU COAL GASIFICATION (LERC)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	0.2 ± 1	Fluorine	0.19 ± .1	Neodymium	0.01 ± 0	Strontium	0.009 ± .001
Antimony	<.008	Gadolinium	<.008	Nickel	<.008	Sulfur	1.3 ± .7
Arsenic	0.02 ± 0	Gallium	<.008	Niobium	<.008	Tantalum	<.008
Barium	0.075 ± .005	Germanium	0.008 ± .001	Osmium	<.008	Tellurium	<.008
Beryllium	<.008	Gold	<.008	Palladium	<.008	Terbium	<.008
Bismuth	<.008	Hafnium	<.008	Phosphorus	0.1 ± 0	Thallium	<.008
Boron	0.03 ± .01	Holmium	<.008	Platinum	<.008	Thorium	<.008
Bromine	<.008	Indium	[illegible]	Potassium	3.6 ± 3.4	Thulium	<.008
Cadmium	<.008	Iodine	<.008	Praseodymium	<.008	Tin	0.02 ± 0
Calcium	2 ± 2	Iridium	<.008	Rhenium	<.008	Titanium	0.12 ± .08
Cerium	<.008	Iron	6 ± 5	Rhodium	<.008	Tungsten	<.008
Cesium	<.008	Lanthanum	<.008	Rubidium	0.005 ± .005	Uranium	<.008
Chlorine	0.5 ± 0	Lead	0.055 ± .015	Ruthenium	<.008	Vandium	0.002 ± 0
Chromium	0.075 ± .025	Lithium	0.004 ± .002	Samarium	<.008	Ytterbium	<.008
Cobalt	0.002 ± .002	Lutetium	<.008	Scandium	0.002 ± 0	Yttrium	<.008
Copper	0.07 ± .03	Magnesium	0.8 ± 0	Selenium	<.008	Zinc	0.035 ± .005
Dysprosium	<.008	Manganese	0.007 ± .002	Silicon	6.6 ± 3.6	Zirconium	0.007 ± .007
Erbium	<.008	Mercury[b]	0.0020	Silver	0.009 ± .009		
Europium	<.008	Molybdenum	0.025 ± .005	Sodium	5 ± 3		

---

[a] Detection limit was 0.008.

[b] Determined by flameless atomic absorption.

Table B42. ELEMENTAL CONCENTRATIONS IN PRODUCT WATER (-19L) FROM WELL 7-8 *IN SITU* COAL GASIFICATION (LERC)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	0.115 ± .085	Fluorine	0.07 ± 0	Neodymium	<.007	Strontium	0.0085 ± .0015
Antimony	<.007	Gadolinium	<.007	Nickel	0.01 ± 0	Sulfur	0.7 ± .3
Arsenic	0.03 ± 1	Gallium	<.007	Niobium	<.007	Tantalum	<.007
Barium	0.075 ± .005	Germanium	≤0.008	Osmium	<.007	Tellurium	<.007
Beryllium	<.007	Gold	<.007	Palladium	<.007	Terbium	<.007
Bismuth	<.007	Hafnium	<.007	Phosphorus	0.1 ± 0	Thallium	<.007
Boron	0.2 ± 0	Holmium	<.007	Platinum	<.007	Thorium	<.007
Bromine	<.007	Indium	[illegible]	Potassium	0.295 ± .20	Thulium	<.007
Cadmium	<.007	Iodine	<.007	Praseodymium	<.007	Tin	0.02 ± 0
Calcium	4 ± 1	Iridium	<.007	Rhenium	<.007	Titanium	0.22 ± .18
Cerium	<.007	Iron	0.5 ± .2	Rhodium	<.007	Tungsten	<.007
Cesium	<.007	Lanthanum	<.007	Rubidium	<.007	Uranium	<.007
Chlorine	0.5 ± 0	Lead	0.045 ± .005	Ruthenium	<.007	Vandium	≤0.002
Chromium	0.04 ± 0	Lithium	0.003 ± .001	Samarium	<.007	Ytterbium	<.007
Cobalt	0.002 ± 0	Lutetium	<.007	Scandium	0.002 ± 0	Yttrium	<.007
Copper	0.05 ± .02	Magnesium	0.9 ± .1	Selenium	<.007	Zinc	0.03 ± 0
Dysprosium	<.007	Manganese	0.015 ± .005	Silicon	1 ± .5	Zirconium	<.007
Erbium	<.007	Mercury[b]	0.0015	Silver	<.007		
Europium	<.007	Molybdenum	0.025 ± .005	Sodium	7 ± 0		

[a] Detection limit was 0.007.

[b] Determined by flameless AA.

Table B43. ELEMENTAL CONCENTRATIONS IN GROUND WATER SAMPLE (CORE HOLE #3) FROM IN SITU COAL GASIFICATION EXPERIMENT (LERC)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	0.28 ± .22	Fluorine	MC	Neodymium	<0.005	Strontium	0.013 ± .006
Antimony	0.006 ± .001	Gadolinium	<0.005	Nickel	0.015 ± .005	Sulfur	MC
Arsenic	0.006 ± .002	Gallium	≤0.003	Niobium	<0.005	Tantalum	<0.005
Barium	0.005 ± .001	Germanium	≤0.006	Osmium	<0.005	Tellurium	<0.005
Beryllium	<0.005	Gold	<0.005	Palladium	<0.005	Terbium	<0.005
Bismuth	<0.005	Hafnium	<0.005	Phosphorus	0.1 ± 0	Thallium	<0.005
Boron	0.06 ± .02	Holmium	<0.005	Platinum	<0.005	Thorium	<0.005
Bromine	0.01 ± 0	Indium	[illegible]	Potassium	4 ± 2	Thulium	<0.005
Cadmium	<0.005	Iodine	≤0.003	Praseodymium	<0.005	Tin	≤0.01
Calcium	5 ± 2	Iridium	<0.005	Rhenium	<0.005	Titanium	0.08 ± .02
Cerium	≤0.003	Iron	7 ± 2	Rhodium	<0.005	Tungsten	<0.005
Cesium	≤0.003	Lanthanum	<0.005	Rubidium	0.014 ± .005	Uranium	<0.005
Chlorine	MC	Lead	0.025 ± .005	Ruthenium	<0.005	Vandium	0.002 ± .001
Chromium	0.006 ± .002	Lithium	0.16 ± .14	Samarium	<0.005	Ytterbium	<0.005
Cobalt	0.001 ± .001	Lutetium	<0.005	Scandium	≤0.005 ± .001	Yttrium	<0.005
Copper	0.03 ± 0	Magnesium	6 ± 1	Selenium	≤0.007	Zinc	0.02 ± 0
Dysprosium	<0.005	Manganese	0.05 ± .04	Silicon	3 ± 1	Zirconium	0.004
Erbium	<0.005	Mercury[b]	0.066	Silver	<0.005		
Europium	<0.005	Molybdenum	≤0.005	Sodium	MC		

[a] Detection limit was 0.005.

[b] Determined by flameless atomic absorption.

Table B44. ELEMENTAL CONCENTRATIONS IN POST-GASIFICATION WATER SAMPLE (WELL#1, HANNA #1) AFTER IN SITU COAL GASIFICATION EXPERIMENT (LERC)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	2 ± 1.9	Fluorine	≃2.8 ± 2.1	Neodymium	0.005	Strontium	0.04 ± .01
Antimony	≤0.005	Gadolinium	<0.005	Nickel	0.03 ± 0	Sulfur	MC
Arsenic	≤0.003	Gallium	≤0.004	Niobium	<0.005	Tantalum	<0.005
Barium	0.015 ± .005	Germanium	<0.005	Osmium	<0.005	Tellurium	<0.005
Beryllium	<0.005	Gold	<0.005	Palladium	<0.005	Terbium	<0.005
Bismuth	<0.005	Hafnium	<0.005	Phosphorus	0.09 ± .01	Thallium	<0.005
Boron	0.3 ± .1	Holmium	<0.005	Platinum	<0.005	Thorium	<0.005
Bromine	0.007 ± .002	Indium	[illegible]	Potassium	1.7 ± 1.2	Thulium	<0.005
Cadmium	<0.005	Iodine	≤0.002	Praseodymium	<0.005	Tin	0.01 ± .01
Calcium	MC	Iridium	<0.005	Rhenium	<0.005	Titanium	0.1 ± 0
Cerium	0.003 ± .001	Iron	1.7 ± 1.4	Rhodium	<0.005	Tungsten	<0.005
Cesium	≤0.003	Lanthanum	≤0.003	Rubidium	0.004 ± .001	Uranium	<0.005
Chlorine	MC	Lead	0.025 ± .005	Ruthenium	<0.005	Vandium	0.002 ± .001
Chromium	0.005 ± .001	Lithium	0.2 ± 0	Samarium	<0.005	Ytterbium	<0.005
Cobalt	0.008 ± .002	Lutetium	<0.005	Scandium	0.006 ± .001	Yttrium	<0.002
Copper	0.05 ± .03	Magnesium	MC	Selenium	0.008 ± .001	Zinc	0.02
Dysprosium	<0.005	Manganese	0.095 ± .005	Silicon	2.8 ± 2.1	Zirconium	≤0.004
Erbium	<0.005	Mercury[b]	0.066	Silver	<0.005		
Europium	<0.005	Molybdenum	≤0.009	Sodium	MC		

[a] Detection limit was 0.005.

[b] Determined by flameless atomic absorption.

Table B45. ELEMENTAL CONCENTRATIONS IN POST-GASIFICATION WATER SAMPLE (WELL #8, HANNA #1) AFTER IN SITU COAL GASIFICATION EXPERIMENT (LERC)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	0.1 ± .05	Fluorine	≈4 ± 1	Neodymium	<0.003	Strontium	0.15 ± 0.05
Antimony	≤0.003	Gadolinium	<0.003	Nickel	0.025 ± .005	Sulfur	MC
Arsenic	0.005 ± .002	Gallium	0.004 ± .002	Niobium	<0.003	Tantalum	<0.003
Barium	0.013 ± .006	Germanium	<0.003	Osmium	<0.003	Tellurium	<0.003
Beryllium	<0.003	Gold	<0.003	Palladium	<0.003	Terbium	<0.003
Bismuth	<0.003	Hafnium	<0.003	Phosphorus	0.09 ± .01	Thallium	<0.003
Boron	0.3 ± .2	Holmium	<0.003	Platinum	<0.003	Thorium	<0.003
Bromine	0.04 ± .01	Indium	S	Potassium	MC	Thulium	<0.003
Cadmium	<0.003	Iodine	≤0.003	Praseodymium	<0.003	Tin	≤0.006
Calcium	MC	Iridium	<0.003	Rhenium	<0.003	Titanium	0.5 ± .1
Cerium	0.003 ± .001	Iron	8 ± 2	Rhodium	<0.003	Tungsten	<0.003
Cesium	≤0.002	Lanthanum	≤0.003	Rubidium	0.05 ± .01	Uranium	<0.003
Chlorine	MC	Lead	0.015 ± .005	Ruthenium	<0.003	Vandium	0.003 ± .002
Chromium	0.004 ± .003	Lithium	3.2 ± 2.8	Samarium	<0.003	Ytterbium	<0.003
Cobalt	0.01 ± .005	Lutetium	<0.003	Scandium	≤0.005	Yttrium	≤0.001
Copper	0.045 ± .005	Magnesium	MC	Selenium	0.007 ± .002	Zinc	0.05 ± .04
Dysprosium	<0.003	Manganese	0.15 ± .05	Silicon	MC	Zirconium	≤0.002
Erbium	<0.003	Mercury[b]	<0.009	Silver	<0.003		
Europium	<0.003	Molybdenum	0.005	Sodium	MC		

[a] Detection limit was 0.003.

[b] Determined by flameless atomic absorption.

Table B46. ELEMENTAL CONCENTRATIONS IN POST-GASIFICATION WATER SAMPLE (WELL-WQ-1) FROM IN SITU COAL GASIFICATION EXPERIMENT (LERC)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	0.03 ± 0	Fluorine	0.35 ± .05	Neodymium	<0.003	Strontium	0.07 ± .02
Antimony	<0.003	Gadolinium	<0.003	Nickel	0.009 ± .001	Sulfur	MC
Arsenic	0.002 ± 0	Gallium	≤0.002	Niobium	<0.003	Tantalum	<0.003
Barium	0.014 ± .006	Germanium	<0.003	Osmium	<0.003	Tellurium	<0.003
Beryllium	<0.003	Gold	<0.003	Palladium	<0.003	Terbium	<0.003
Bismuth	<0.003	Hafnium	<0.003	Phosphorus	0.08 ± .04	Thallium	<0.003
Boron	0.08 ± .02	Holmium	<0.003	Platinum	<0.003	Thorium	<0.003
Bromine	0.004 ± .001	Indium	[illegible]	Potassium	MC	Thulium	<0.003
Cadmium	<0.003	Iodine	≤0.001	Praseodymium	<0.003	Tin	<0.003
Calcium	MC	Iridium	<0.003	Rhenium	<0.003	Titanium	0.05 ± .01
Cerium	≤0.002	Iron	0.6 ± .3	Rhodium	<0.003	Tungsten	<0.003
Cesium	≤0.001	Lanthanum	≤0.001	Rubidium	0.005 ± .004	Uranium	<0.003
Chlorine	5 ± 1	Lead	≤0.01	Ruthenium	<0.003	Vandium	0.001 ± 0
Chromium	0.003 ± 0	Lithium	0.2 ± 0	Samarium	<0.003	Ytterbium	<0.003
Cobalt	0.001 ± .001	Lutetium	<0.003	Scandium	0.003 ± .001	Yttrium	<0.003
Copper	0.005 ± .001	Magnesium	5 ± 1	Selenium	<0.003	Zinc	0.009 ± .001
Dysprosium	<0.003	Manganese	0.05 ± .03	Silicon	3 ± 1	Zirconium	0.004 ± .002
Erbium	<0.003	Mercury[b]	0.011	Silver	<0.003		
Europium	<0.003	Molybdenum	≤0.006	Sodium	7 ± 1		

---

[a] Detection limit was 0.003.

[b] Determined by flameless atomic absorption.

Table B47. ELEMENTAL CONCENTRATIONS IN POST-GASIFICATION WATER SAMPLE (WELL #1, HANNA #2) FROM IN SITU COAL GASIFICATION EXPERIMENT (LERC)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	0.5 ± .1	Fluorine	MC	Neodymium	<0.004	Strontium	<0.004
Antimony	0.005 ± .001	Gadolinium	<0.004	Nickel	<0.004	Sulfur	MC
Arsenic	<0.004	Gallium	<0.004	Niobium	<0.004	Tantalum	<0.004
Barium	0.03 ± 0	Germanium	<0.004	Osmium	<0.004	Tellurium	<0.004
Beryllium	<0.004	Gold	<0.004	Palladium	<0.004	Terbium	<0.004
Bismuth	0.012 ± .010	Hafnium	<0.004	Phosphorus	0.3 ± .1	Thallium	<0.004
Boron	0.6 ± .2	Holmium	<0.004	Platinum	<0.004	Thorium	<0.004
Bromine	<0.004	Indium	[illegible]	Potassium	2.5 ± .5	Thulium	<0.004
Cadmium	0.017 ± .017	Iodine	0.003 ± 0	Praseodymium	<0.004	Tin	0.009 ± .001
Calcium	MC	Iridium	<0.004	Rhenium	<0.004	Titanium	0.15 ± .05
Cerium	0.003 ± .001	Iron	<0.004	Rhodium	<0.004	Tungsten	<0.004
Cesium	0.002 ± 0	Lanthanum	0.002 ± .002	Rubidium	<0.004	Uranium	<0.004
Chlorine	MC	Lead	0.095 ± .005	Ruthenium	<0.004	Vandium	0.003 ± .001
Chromium	<0.004	Lithium	0.21 ± .2	Samarium	<0.004	Ytterbium	<0.004
Cobalt	<0.004	Lutetium	<0.004	Scandium	0.006 ± .001	Yttrium	<0.004
Copper	<0.004	Magnesium	MC	Selenium	<0.004	Zinc	<0.004
Dysprosium	<0.004	Manganese	<0.004	Silicon	5.5 ± .5	Zirconium	<0.004
Erbium	<0.004	Mercury[b]	<0.009	Silver	0.005 ± .001		
Europium	<0.004	Molybdenum	<0.004	Sodium	MC		

[a] Detection limit was 0.004.

[b] Determined by flameless atomic absorption.

Table B48. ELEMENTAL CONCENTRATIONS IN POST-GASIFICATION WATER SAMPLE (WELL #4, HANNA #2) FROM IN SITU COAL GASIFICATION EXPERIMENT (LERC)

Element	ppm[a]	Element	ppm	Element	ppm	Element	ppm
Aluminum	0.26 ± .24	Fluorine	1.8 ± 1.2	Neodymium	<0.004	Strontium	0.085 ± .005
Antimony	≤0.005	Gadolinium	<0.004	Nickel	0.025 ± .005	Sulfur	MC
Arsenic	0.003 ± .001	Gallium	0.004 ± 0	Niobium	0.09 ± .09	Tantalum	0.004
Barium	0.04 ± 0	Germanium	<0.004	Osmium	<0.004	Tellurium	0.004
Beryllium	<0.004	Gold	<0.004	Palladium	<0.004	Terbium	0.004
Bismuth	<0.004	Hafnium	<0.004	Phosphorus	0.08 ± .02	Thallium	0.004
Boron	0.15 ± .05	Holmium	<0.004	Platinum	<0.004	Thorium	0.004
Bromine	0.015 ± .005	Indium	[illegible]	Potassium	8 ± 0	Thulium	0.004
Cadmium	<0.004	Iodine	0.003 ± .003	Praseodymium	<0.004	Tin	0.01
Calcium	MC	Iridium	<0.004	Rhenium	<0.004	Titanium	0.1 ± 0
Cerium	0.004 ± .001	Iron	5.5 ± .5	Rhodium	<0.004	Tungsten	0.004
Cesium	≤0.003	Lanthanum	≤0.003	Rubidium	0.010 ± .008	Uranium	0.004
Chlorine	4 ± 1	Lead	≤0.02	Ruthenium	<0.004	Vandium	0.003 ± .001
Chromium	0.008 ± .002	Lithium	0.15 ± .05	Samarium	<0.004	Ytterbium	0.004
Cobalt	0.005 ± .004	Lutetium	<0.004	Scandium	≤0.009	Yttrium	0.004
Copper	0.02 ± 0	Magnesium	6 ± 0	Selenium	0.008 ± .002	Zinc	0.02 ± 0
Dysprosium	<0.004	Manganese	0.3 ± .1	Silicon	2.5 ± 1.5	Zirconium	0.007 ± .003
Erbium	<0.004	Mercury[b]	<0.009	Silver	<0.004		
Europium	<0.004	Molybdenum	0.02 ± .01	Sodium	MC		

[a] Detection limit was 0.004.

[b] Determined by flameless atomic absorption.

APPENDIX C

VOLATILE ORGANIC SUBSTANCES IN LIQUID AND SOLID EFFLUENTS FROM ENERGY-RELATED PROCESSES

		Page
Part I:	Samples from Oil-Shale Processing.	286
Part II:	Samples from Low Btu Gasification of Rosebud Coal. .	295
Part III:	Samples from In Situ Coal Gasification in Gillette, WY	311
Part IV:	Samples from In Situ Coal Gasification in Hanna, WY.	354

Reproduced from best available copy.

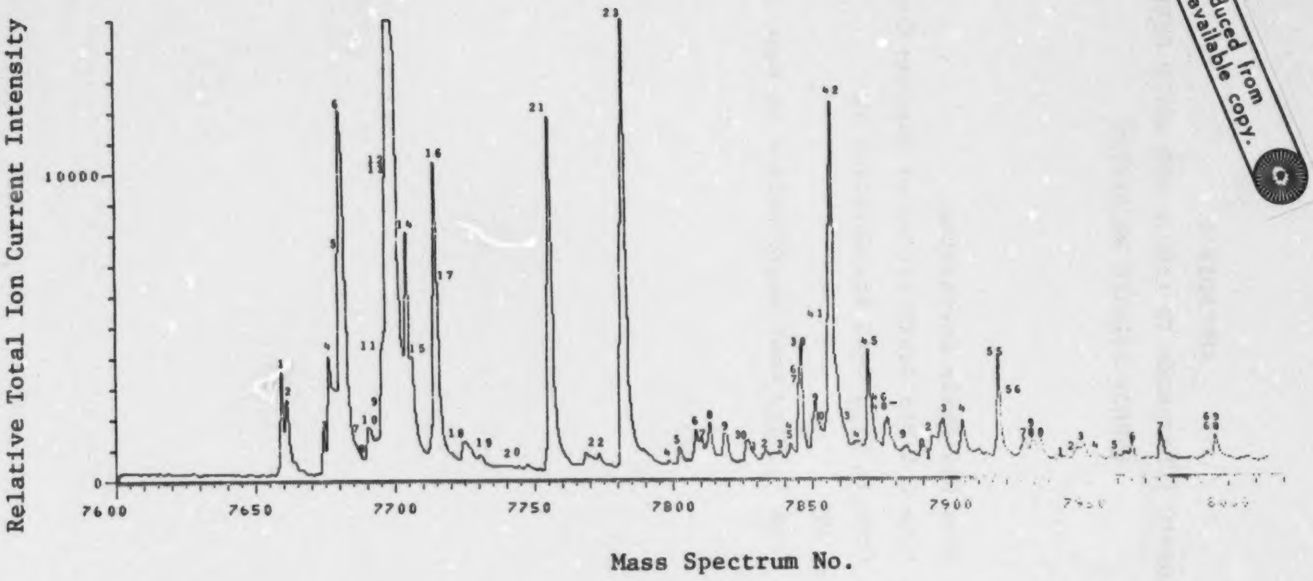


Figure C1. Profile of volatile organics in aqueous sample from 150 Ton oil-shale retort (LERC, ERDA).

Table C1. VOLATILE ORGANICS IN AQUEOUS SAMPLE FROM 150 TON OIL-SHALE RETORT PROCESSING (LERC, ERDA)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
2	105	acetone	200±56
3	105	*n*-pentane	10±3
4	106	diethyl ether	13±9
6	107	*t*-butanol	130±91
7	108	nitromethane	16±7
8	109	methoxy-1-butene (tent.)	6±5
8A	110	cyanoethane (tent.)	53±21
9	111	3-methylpentane	13±2
10	115	*n*-hexane	53±5
12	123	methyl ethyl ketone (tent.)	6±1
13	128	methylcyclopentane	680±5.0
15	131	2-methylbutan-2-ol	17±3
16	133	benzene	14.5±7
17	134	thiophene	8±4
17A	138	cyclohexane	5±3
18	139	isobutyronitrile	9±1
20	148	*n*-heptane	10±2
21	153	*N*-methylpyrazole	177±20
22	162	2,3-dimethylbutan-2-ol or *n*-propyl *t*-butyl ether	trace
23	164	toluene	300±100
25	172	1-methylthiophene	9±7
26	173	pyridine	4±1
27	174	phenol	2±0.5
28	175	ethylbenzene	11±2
29	176	*p*-xylene	28±6
29A	177	*m*-xylene	24±6
30	177	1,4-dimethylthiophene (tent.)	9±2
31	178	thiacyclohexane	22±6
32	179	*o*-xylene	7±1
33	181	methylthiacyclohexane isomer	trace
34	184	methylpyridine isomer (tent.)	9±2
35	190	*n*-propylbenzene	40±15
36	192	ethyltoluene isomer	24±8
37	194	ethyltoluene isomer	23±9
39	200	C_3-alkyl benzene isomer	80±22
40	201	unknown	NQ
41	203	dimethylindene isomer (tent.)	2±2
43	209	C_3-alkyl benzene isomer	4±1
44	212	*o*-methylphenol	10±5
45	215	2,2,6-trimethylcyclohexanone	9.5±1
46	220	C_4-alkyl benzene isomer	3.2±5
47	225	acetophenone	2.7±0.4
48	229	C_4-alkyl benzene isomer	4.6±0.6
49	230	unknown	NQ
50	230	*p*-methylphenol	4±1
51	233	C_4-alkyl benzene isomer	8±1
52	236	*o*-ethyltoluene	17±3
53	237	4,5-dihydroxyheptane	68±21
54	240	*m*-ethylphenol	12±3
55	↓	C_4-alkyl benzene isomer	trace
56	↓	unknown (aromatic)	NQ
57	↓	naphthalene	75±32
58	↓	dimethylbenzofuran isomer	3.6±0.3
59	↓	methylbenzocyclopentenone	4.2±0.3
60	↓	unknown	NQ
61	↓	β-methylnaphthalene	61±10
62	↓	α-methylnaphthalene	52±17

Table C2. VOLATILE ORGANICS IN AQUEOUS BOILER BLOW-DOWN SAMPLE FROM *IN SITU* OIL-SHALE PROCESSING (OCC)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
1	43	CO_2	NQ
2	45	methyl ethyl ether	5.46±2.1
2A	46	acetaldehyde	2.75±1.1
2C	49	isopentane	T
3A	51	*n*-pentane	T
4	51	acetone + diethyl ether	48.0±16
6	57	2-methylpentane	3.40±1.1
7	59	3-methylpentane	18.3±6.6
8	61	hexafluorobenzene (eS) + *n*-hexane	51.0±21
8B	64	methyl ethyl ketone	T
9	65	methylcyclopentane + perfluorotoluene (eS)	27.9±5.7
9C	69	C_7H_{16} isomer	T
10	70	benzene	4.1±1.3
10B	71	cyclohexane	T
10C	72	C_7H_{16} isomer	T
12	76	C_8H_{18} isomer	48.2±26
12A	78	$C_5H_{10}O$ isomer (tent.)	9.85±1.9
12B	78	*n*-heptane	19.2±2.7
13	80	$C_5H_{10}O$ alcohol isomer (tent.)	NQ
13A	83	C_7H_{14} isomer	T
13B	84	*n*-hexanal (tent.)	T
14	90	toluene	19.2±6
14A	94	C_8H_{16} isomer	T
15C	107	C_8H_{16} isomer	T
15D	112	ethylbenzene	T
16	113	*p*-xylene	T
17	116	$C_{10}H_{22}$ isomer	6.89±1.4
17A	116	styrene	T
18	117	$C_{10}H_{22}$ isomer	10.2±3.7
18A	118	C_9H_{18} isomer	T
18B	118	$C_7H_{14}O$ isomer	T
19	119	*n*-nonane or C_9H_{20} isomer	3.43±0.7
19A	121	$C_{10}H_{20}$ isomer	T
20	123	$C_{10}H_{22}$ isomer	17.10±3.7
20A	124	$C_{11}H_{24}$ isomer	4.14±0
20B	125	$C_{10}H_{20}$ isomer	T
21	126	$C_{10}H_{22}$ isomer	7.49±2.5
21A	128	$C_{10}H_{20}$ isomer	T
22	129	$C_{10}H_{22}$ + C_3-alkyl benzene isomers	1.78±0.4
23	131	$C_{11}H_{24}$ isomer	31.8±27
24	133	$C_{11}H_{24}$ isomer	27.2±21
25	135	$C_{11}H_{24}$ isomer	5.53±5
25A	136	C_3-alkyl benzene isomer	T
26	137	*n*-decane	5.53±1.7
27	138	phenol + $C_{10}H_{20}$ isomer	NQ
27A	139	$C_{11}H_{24}$ isomer	T
28	141	$C_{11}H_{24}$ isomer	7.67±2.9
29	142	$C_{12}H_{26}$ isomer	3.96±2.1
30	144	$C_{10}H_{20}$ isomer	1.96±0.5
31	145	$C_{13}H_{28}$ isomer	7.17±6.1
31	146	$C_{12}H_{24}$ isomer	T
32	148	hydrocarbon	NA
33	150	acetophenone	T
33A	150	C_4-alkyl benzene isomer	T
33B	152	cresol isomer	NQ
34	153	$C_{11}H_{24}$ isomer	T
35	154	*n*-undecane	0.89±0.5
35A	157	$C_{11}H_{22}$ + cresol isomers	T
36	162	dimethylphenol isomer	NQ
37	166	dimethylphenol isomer	NQ
37A	168	naphthalene	T
38	170	$C_{12}H_{24}$ isomer	T
39	171	*n*-dodecane	0.37±0.1
39A	175	C_3-alkyl phenol isomer	NQ
39B	175	C_2-alkyl phenol isomer	NQ
39C	176	C_3-alkyl phenol isomer	NQ
39D	181	C_3-alkyl phenol isomer	NQ
39E	184	$C_{13}H_{26}$ isomer	T
40	185	*n*-tridecane	0.89±0.5
41	188	C_3-alkyl phenol + methylnaphthalene + C_5-alkyl phenol isomers	NQ
42	196	C_4-alkyl phenol + $C_{14}H_{28}$ isomers	NQ
43	199	*n*-tetradecane	1.96±0.7
44	203	C_2-alkyl naphthalene isomer	T
45	206	$C_{15}H_{30}$ isomer	T
46	208	$C_{15}H_{32}$ isomer	T
47	211	$C_{15}H_{30}$ isomer	T
48	213	*n*-pentadecane	5.53±2.6
48A	214	C_3-alkyl naphthalene isomer	T
48B	218	C_3-alkyl naphthalene isomer	T
49	220	$C_{15}H_{30}$ isomer	T
51	224	alkyl butanoic acid isomer (tent.)	NQ
52	225	*n*-hexadecane	7.67±3.9
52A	226	$C_{16}H_{32}$ isomer	1.96±0.9
53A	232	$C_{17}H_{34}$ isomer	T
54	237	*n*-heptadecane	9.17±8.2

Table C3. VOLATILE ORGANICS IN OMEGA-9 RETORT WATER FROM *IN SITU* OIL-SHALE PROCESSING PRIOR TO INCUBATION AT 75°F (LERC, ERDA)

Chromatographic Peak No.	Elution Temp. (°C)	Compound	ppb
1	41	CO_2	-
2A	44	butene isomer	NQ
2B	47	isopentane	4.2±2
3	49	acetone	126.3±40
4	51	acetonitrile	42.0±11
4A	55	isopropanol	22.8±6
5	56	ter-butanol	17.5±7
6	58	propionitrile + hexafluorobenzene (eS)	27.3±7
6A	58	*n*-hexane	2.8±1.4
7	59	methyl ethyl ketone	75.8±3.4
8	63	perfluorotoluene (eS)	
8A	65	isobutyronitrile	3.0±1.5
9	67	benzene	133.9±3
9A	68	thiophene	19.6±6.4
10	68	methyl isopropyl ketone	20.2±12
11	71	*n*-butyronitrile	13±3.4
12	72	2-pentanone	197±72
13	75	3-pentanone	26±14
13A	79	$C_6H_{12}O$ isomer	12.6±4
13B	81	α-methylbutyronitrile	30.3±14
14	82	4-methyl-2-pentanone	105±70
15	85	2-methyl-3-pentanone	62±30
15A	86	3-methyl-2-pentanone	12±2.5
15B	87	pyrrole	22.7±15
16	87	toluene	6.7±1.1
16A	88	2-methylthiophene	T
16B	90	3-methylthiophene	T
17	91	*n*-pentylnitrile	10.9±4
18	92	3-hexanone	5.3±17
19	93	2-hexanone	52.6±22
19A	95	thiacyclopentane	5.6±2.8
20	97	cyclopentanone	5.0±2.9
20A	97	4-methylpentylnitrile	T
21	99	pyridine	152±62
21A	99	3-methylisothiazole	6.8±1.1
21C	100	acetoxy-2-butene or $C_6H_{10}O_2$ isomer	NQ
22	101	5-methyl-3-hexanone	T
23	102	2-methyl-3-hexanone	T
23A	102	2-methylcyclopentanone	7.7±2.7
23B	103	$C_7H_{14}O$ isomer	18.9±6.2
24	103	2-methylthiacyclopentane	3±0.2
24A	104	$C_6H_{10}O_2$ isomer	14.7±8.8
24B	104	5-methyl-2-hexanone	T
25	106	$C_7H_{14}O$ isomer	18.7±1.5
25A	107	ethylbenzene	2.1±1
26	107	$C_7H_{12}O$ or C_8H_{16} isomer	T
27	108	2-methylpyridine + *m*-xylene	40.5±6.7
27A	109	4-heptanone	T
27B	109	3-methylpyridine + *n*-hexylnitrile	16.5±6
27C	110	dimethylthiacyclopentane isomer	0.34±0.2
28	110	thiacyclohexane	4.6±2
28A	111	2,5-dimethylthiacyclopentane	3.5±1.5
28B	111	$C_7H_{12}O$ isomer	T
29	112	3-heptanone	28±18
30	113	2-heptanone	244±100
30A	113	*o*-xylene	5.6±2.8
31	115	C_9H_{18} isomer	3.2±1.5
32	117	$C_8H_{14}O$ isomer	1.2±0.3
33	118	dimethylpyridine isomer	16.4±6.2
34	119	C_9H_{20} isomer (tent.)	T
35	120	methylthiacyclohexane + $C_8H_{14}O$ isomers (tent.)	T
35A	121	$C_8H_{14}O$ isomer + 3-methylcyclohexanone	0.96±0.2
35B	121	$C_8H_{16}O$ isomer	T
36	122	2-ethylpyridine	T
36A	124	2-methylcyclohexanone	T
36B	124	3-octanone	T
37	125	2-octanone	126±42
38	127	aniline + C_2-alkyl pyridine isomer	45.4±6.8
38A	127	C_3-alkyl pyridine isomer	15±4.4
39	128	C_2-alkyl pyridine isomer + *n*-heptylnitrile	35±12.5
40	129	C_3-alkyl pyridine isomer	63±14
41	130	cyanobenzene	235±155
42	131	C_7H_9N + $C_7H_{10}O_2$ (tent.) isomers	NQ
42A	132	$C_8H_{16}O$ isomer	13.1±0.4
43	133	$C_9H_{16}O$ isomer	25.3±10
43A	134	C_4-alkyl pyridine isomer	NQ
44	135	2,4,6-trimethylpyridine	T
45	140	trimethylcyclohexanone isomer	0.7±0.3
46	141	C_3-alkyl cyclohexanone isomer	T
46A	142	C_4-alkyl pyridine isomer	T
46B	144	$C_8H_{12}O$ isomer (tent.)	19.3±5
47	144	$C_9H_{18}O$ isomer	1.36±0.7
47A	145	trimethylcyclohexanone	T
47B	146	benzylcyanide or tolunitrile	10.8±5.2

(continued)

Table C3 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb	Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
47C	147	$C_9H_{16}O$ isomer	T			
48	147	C_4-alkyl pyridine isomer	T			
49	150	$C_9H_{18}O$ isomer	21.9±12			
50	151	C_4-alkyl pyridine isomer	NQ			
51	153	C_5-alkyl pyridine isomer				
51A	155	C_4-alkyl pyridine isomer				
52	156	C_5-alkyl pyridine isomer	11±6			
52A	157	$C_{10}H_{18}O$ isomer	T			
53	159	C_5-alkyl pyridine isomer	19±8			
54	160	$C_{10}H_{18}O$ isomer	T			
54A	160	1,3,5-trimethylpyrazole	14±6			
55	161	C_5-alkyl pyridine isomer	4.2±2			
56	162	$C_9H_{13}N$ isomer	T			
57	163	C_6-alkyl pyridine isomer	NQ			
58	165	$C_9H_{13}N$ isomer	NQ			
59	166	$C_{11}H_{20}O$ or $C_{10}H_{16}O_2$ isomer	T			
60	167	naphthalene	29±18			
61	168	C_6-alkyl pyridine isomer	NQ			
61A	169	$C_9H_{13}N$ isomer	T			
62	171	C_5-alkyl pyridine isomer	NQ (trace)			
63	172	C_6-alkyl pyridine isomer				
64	174	C_6-alkyl pyridine isomer				
65	176	C_7-alkyl pyridine isomer				
66	178	C_6-alkyl pyridine isomer				
66A	179	$C_{14}H_{30}$ isomer	4.2±2.1			
67	180	C_7-alkyl pyridine isomer	NQ			
68	182	quinoline	18.6±7.5			
69	183	n-tridecane	8.4±2.4			
70	185	alkyl pyridine isomer	NQ (trace)			
71	189	$C_{10}H_{15}N$ isomer				
72	191	C_8-alkyl pyridine isomer				
73	192	alkyl pyridine isomer				
74	195	$C_{15}H_{32}$ isomer	6.7±2.2			
75	197	n-tetradecane				
75A	198	$C_{15}H_{30}$ isomer	T			
76	222	$C_{14}H_{28}O$ isomer	1.9±0.3			
76A	223	n-hexadecane	0.7±0.3			
77	235	$C_{15}H_{30}O$ isomer	T			
78	236	n-heptadecane	0.6±0.4			

Table C4. VOLATILE ORGANICS IN OMEGA-9 RETORT WATER FROM *IN SITU* OIL-SHALE PROCESSING AFTER INCUBATION AT 75°F FOR 2 MONTHS (LERC, ERDA)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
1	41	CO_2	-
1A	45	butene isomer (tent.)	NQ
2	50	acetone	95±44
2A	51	acetonitrile	23±11
2C	51	isopropanol	9±4
3	58	ter-butanol	8.5±2.5
4	60	propionitrile	10±4
5	61	methyl ethyl ketone + hexafluorobenzene (eS)	152±67
6	66	perfluorotoluene (eS)	
6A	69	isobutyronitrile	1.1±0.4
7	71	benzene	37±18
7A	71	thiophene	4.6±3
8	72	methyl isopropyl ketone	9.6±4.8
9	76	*n*-butyronitrile	NQ
10	77	2-pentanone	123±42
10A	78	3-pentanone	11±6
11	85	α-methylbutyronitrile	5±3
12	86	4-methyl-2-pentanone	51±20
13	88	2-methyl-3-pentanone	11.3±1.9
14	90	3-methyl-2-pentanone + pyrrole + toluene	0.4±0.2
15	94	*n*-pentylnitrile	5.0±2
16	94	3-hexanone	12.8±6.2
17	95	2-hexanone	38±14
17A	97	thiacyclopentane	1.9±0.9
18	97	cyclopentanone	2.9±1.4
18A	98	4-methylpentylnitrile	NQ
19	99	pyridine	185±121
20	102	3-methyl acetylacetone	T
21	103	5-methyl-3-hexanone	T
21A	104	2-methyl-3-hexanone	T
22	104	2-methylcyclopentanone	T
23	105	2-methylthiacyclopentane + $C_6H_{10}O_2$ isomer	NQ
23A	106	$C_7H_{14}O$ isomer	5.1±2.5
24	106	2-methylpyridine	17.8±8.8
25	108	$C_7H_{14}O$ isomer	3.8±1.8
26	109	C_8H_{16} *or* $C_7H_{12}O$ isomer	4±1
27	110	4-heptanone	8.2±4
28	111	*n*-hexylnitrile	5.9±2.4
29	112	dimethylthiacyclopentane isomer	NQ
29A	112	$C_7H_{12}O$ isomer	43±10
30	113	3-heptanone	30±24
31	114	2-heptanone	52±18
31A	116	$C_8H_{14}O$ isomer	T
32	116	C_2-alkyl pyridine isomer	240±32
33	118	C_2-alkyl pyridine isomer	
34	119	C_2-alkyl pyridine isomer	
35	121	$C_8H_{14}O$ isomer	T
35A	121	$C_7H_{12}O$ isomer	T
36	122	$C_8H_{16}O$ isomer	0.96±0.2
37	123	C_2-alkyl pyridine isomer	T
38	124	2-methylcyclohexanone	T
39	125	2-octanone	19±12
40	125	aniline	17±8
40A	126	C_3-alkyl pyridine isomer	T
41	126	C_2-alkyl pyridine isomer	2.5±1.2
41A	128	*n*-heptylnitrile (tent.)	T
41B	128	$C_8H_{14}O$ isomer	T
42	129	C_3-alkyl pyridine isomer	14.2±5
43	131	cyanobenzene	49±20
44	132	$C_8H_{16}O$ + $C_8H_{14}O$ isomers	18±4.8
45	133	$C_9H_{16}O$ isomer	0.5±0.3
46	134	C_3-alkyl pyridine isomer	0.5±0.2
46A	135	C_4-alkyl pyridine isomer	T
47	139	C_3-alkyl pyridine isomer	NQ
48	140	trimethylcyclohexanone isomer	0.6±
49	141	C_4-alkyl pyridine isomer	NQ
50	143	$C_8H_{14}O$ isomer (tent.)	T
50A	144	$C_8H_{10}O_2$ isomer (tent.)	T
51	145	C_7H_9N isomer	NQ
52	148	C_4-alkyl pyridine isomer	5.7±2.8
53	154	C_5-alkyl pyridine isomer	5.1±2.7
55	193	$C_{12}H_{24}O_3$ isomer	NQ

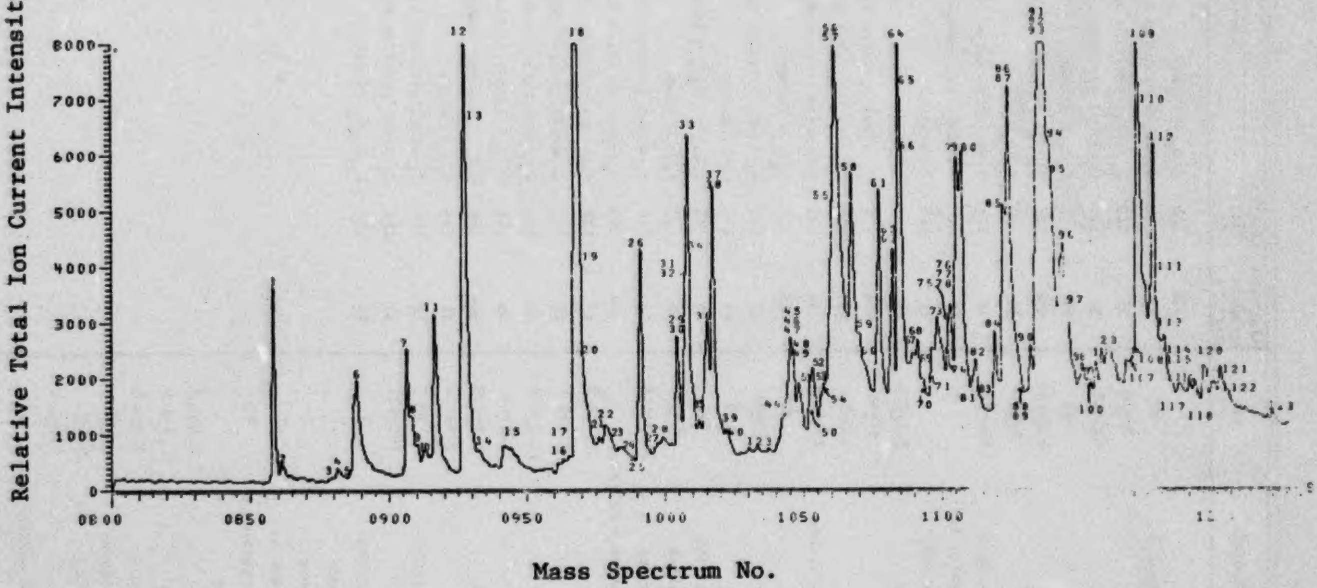


Figure C2. Profile of volatile organics in aqueous condensate (-1L) from low btu gasification of Rosebud coal (MERC, ERDA).

Table C5. VOLATILE ORGANICS IN AQUEOUS CONDENSATE (-1L) FROM LOW BTU GASIFICATION OF ROSEBUD COAL (MERC, ERDA)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
1	50	CO_2	-
4	63	acetaldehyde	28.6
5	64	C_4H_{10} isomer	NQ
7	75	perfluorobenzene (e[illegible])	
8	75	*n*-hexane	21.4
10	77	methyl ethyl ketone	14.2
11	79	perfluorotoluene (e[illegible])	
12	85	benzene	623
13	85	thiophene	T
14	88	C_6H_{14} isomer	T
15	92	C_6H_{14} isomer	T
16	102	C_7H_{16} isomer	T
17	103	C_7H_{16} isomer	13
18	105	toluene isomer	706
19	106	methylthiophene isomer	38.8
20	107	methylthiophene isomer	37.4
21	109	C_7H_{16} isomer	T
22	111	C_7H_{16} isomer	6.0
23	112	C_7H_{16} isomer	8.8
24	114	C_7H_{14} isomer	T
25	115	C_7H_{14} isomer	T
26	119	C_8H_{18} isomer	T
28	121	pyridine	95.2
29	123	ethylbenzene	57.6
30	123	C_8H_{16} isomer	T
31	124	*p*-xylene + *m*-xylene	57.2
32	124	C_8H_{16} isomer	4
33	124	phenylacetylene	17.2
34	127	dimethylthiophene isomer	9.8
35	128	C_8H_{18} isomer	31
36	129	styrene or cyclooctatetraene	85.6
37	130	C_8H_{16} isomer	T
38	134	*o*-xylene	133.4
39	134	C_8H_{18} isomer	6.2
40	134	anisole	3.8
41	136	benzaldehyde	38.0
42	140	C_9H_{20} isomer	T
43	142	methylstyrene isomer	T
44	144	C_3-alkyl benzene isomer	222
45	144	C_3-alkyl benzene isomer	26
46	144	C_9H_{18} isomer	T
47	144	C_3-alkyl benzene isomer	23.4
48	145	C_9H_{18} isomer	T
49	146	C_9H_{20} isomer	T
50	147	cyanobenzene	8.2
51	148	C_3-alkyl benzene isomer	4.0
52	148	C_9H_{18} isomer	3.0
53	149	C_9H_{20} isomer	T
54	150	methylstyrene isomer	T
55	151	aniline	1143
56	152	benzofuran	171
57	152	C_3-alkyl benzene isomer	T
59	156	$C_{10}H_{22}$ isomer	4.0
60	157	C_9H_{18} isomer	4.4
61	160	C_4-alkyl	6.4
62	162	indan	114
63	162	dimethylstyrene isomer	T
64	164	indene	375
65	164	C_4-alkyl benzene isomer	9.0
66	165	$C_{10}H_{20}$ isomer	11.0
67	166	C_4-alkyl benzene isomer	12.0
68	167	$C_{10}H_{22}$ isomer	T
69	168	$C_{10}H_{20}$ isomer	T
70	169	C_4H_7-benzene isomer	13.2
71	169	nitrobenzene	37.2
72	170	$C_{10}H_{22}$ isomer	3.0
73	171	C_4-alkyl benzene	T
74	173	C_4H_7-benzene isomer	T
75	173	methylbenzofuran isomer	38
76	173	$C_{11}H_{24}$ isomer	T
77	173	C_5-alkyl benzene isomer	40
78	173	$C_{11}H_{22}$ isomer	35
79	174	methylbenzofuran isomer	176
80	175	C_4-alkyl benzene isomer	T
81	177	methylbenzofuran isomer	57.2
82	178	C_5-alkyl benzene isomer	T
83	179	$C_{11}H_{20}$ isomer	T
84	181	methylindan isomer	34.2
85	183	methylindene isomer	98
86	183	C_4H_7-benzene isomer	21
87	183	C_5-alkyl benzene isomer	22
88	186	C_5-alkyl benzene isomer	23
89	186	methylanisole isomer	9.6
90	188	$C_{11}H_{24}$ isomer	6.4
91	189	naphthalene	914
92	190	C_4-alkyl benzene isomer	T
93	191	dimethylindan isomer	T
94	192	$C_{12}H_{26}$ isomer	T
95	192	dimethylindan isomer	91
96	193	dimethylbenzofuran isomer	91
97	194	C_6-alkyl benzene isomer	T
98	197	dimethylindan isomer	22.8

(continued)

Table C5 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb	Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
99	198	C_6-alkyl benzene isomer	T				
100	199	C_6H_{11}-benzene isomer	T				
101	200	dimethylindan isomer	22.8				
102	200	naphthol	37.6				
103	201	$C_{12}H_{26}$ isomer	T				
104	202	dimethylindan isomer	11.4				
105	204	C_6H_{11}-benzene isomer	T				
106	205	dimethylindole isomer	18.2				
107	206	C_6H_{11}-benzene isomer	T				
108	206	C_6-alkyl benzene isomer	T				
109	207	β-methylnaphthalene	3162				
110	208	C_6H_{11}-benzene isomer	T				
111	209	methylbenzothiophene (tent.)	T				
112	210	α-methylnaphthalene	248				
113	211	C_6H_{11}-benzene isomer	T				
114	212	C_7H_{13}-benzene isomer	T				
115	212	C_7-alkyl benzene isomer	21				
116	214	C_7H_{13}-benzene isomer	T				
117	215	C_7H_{13}-benzene isomer	T				
118	216	$C_{14}H_{26}$ isomer	T				
119	219	biphenyl	38				
120	221	C_7H_{13}-benzene isomer	T				
121	222	$C_{11}H_{24}$ isomer	T				
122	223	C_8-alkyl benzene isomer	T				
123	232	diphenoxybenzene	T				

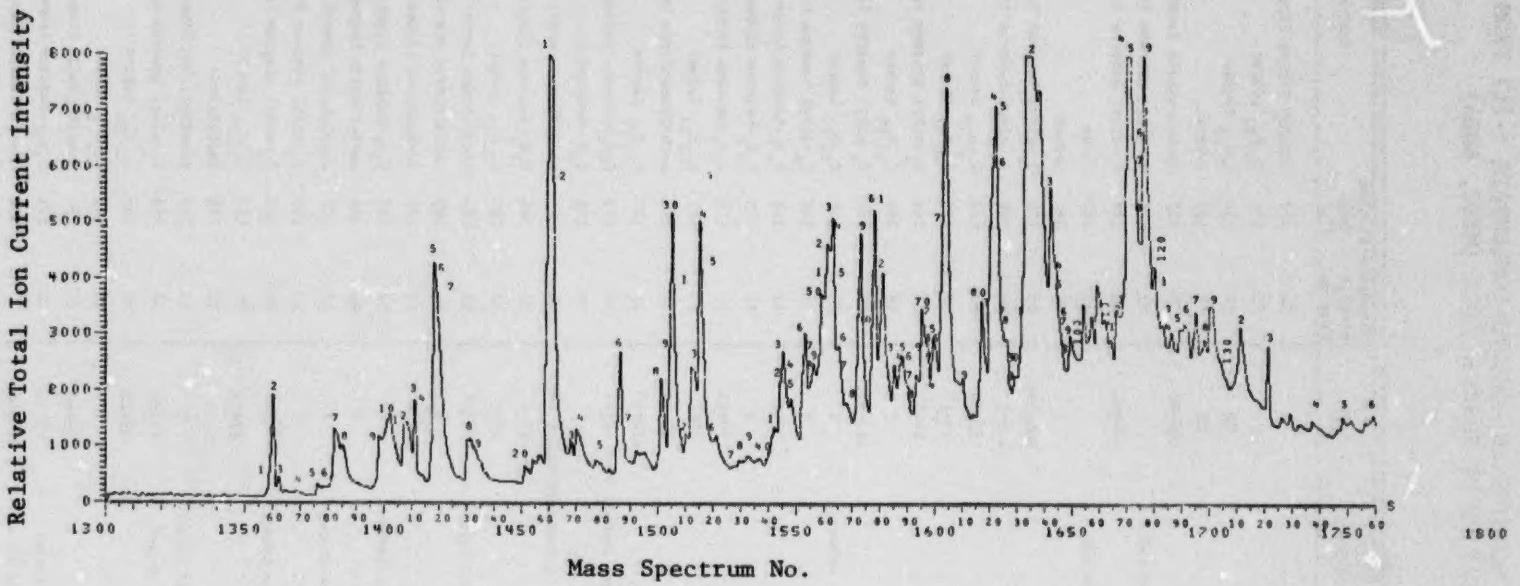


Figure C3. Profile of volatile organics in aqueous condensate (-2L) from low btu gasification of coal (MERC, ERDA).

Table C6. VOLATILE ORGANICS IN AQUEOUS CONDENSATE (-2L) FROM LOW BTU GASIFICATION OF ROSEBUD COAL (MERC, ERDA)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
1	49	$N_2 + O_2$	-
2	50	CO_2	-
4	54	C_4H_8 isomer	NQ
6	59	C_4H_{10} isomer	NQ
8	63	acetone	100±20
9	70	perfluorobenzene (eS)	
10	71	C_5H_{12} isomer	154±66
12	74	perfluorotoluene (eS)	
14	77	C_5H_{12} isomer	T
15	79	benzene	308±134
16	81	thiophene	4.5±1
17	81	C_6H_{14} isomer	57±10
18	85	C_6H_{14} isomer	90±17
19	87	C_6H_{14} isomer	84±33
20	96	C_7H_{16} isomer	T
21	100	toluene	381±83
22	101	methylthiophene isomer	T
23	104	C_7H_{16} isomer	T
24	106	C_7H_{16} isomer	33±17
25	110	C_7H_{14} isomer	T
27	116	C_8H_{18} isomer	20±13
28	121	ethylbenzene	38±7
29	123	C_8H_{16} isomer	40±20
30	124	m- and p-xylene	210±67
31	124	dimethylthiophene isomer	32±24
32	126	C_8H_{18} isomer	T
33	127	styrene and/or cyclooctatetraene	12±3
34	128	o-xylene	16±8
35	129	C_8H_{16} isomer	23±5
36	131	dimethylthiophene isomer	47±10
37	132	C_9H_{20} isomer	T
38	133	anisole	4.6±1.4
39	136	C_3-alkyl benzene isomer	T
40	137	C_9H_{20} isomer	T
41	141	C_3-alkyl benzene isomer	T
42	143	benzaldehyde	T
43	143	C_3-alkyl benzene isomer	107±10
44	144	C_9H_{18} isomer	67±33
45	144	C_9H_{20} isomer	
46	147	C_3-alkyl benzene isomer	T
47	147	methylpyridine isomer	47±10
48	148	C_9H_{18} isomer	33±20
49	148	C_9H_{20} isomer	T
50	149	benzofuran	59±40
51	149	methylpyridine isomer	38±11
52	150	C_3-alkyl benzene isomer	144±18
54	152	methylpyridine isomer	16±7
55	154	$C_{10}H_{22}$ isomer	T
56	154	C_9H_{18} isomer	T
57	155	unknown	T
58	155	methylanisole isomer	T
59	158	C_4-alkyl benzene isomer	301±104
60	158	C_4-alkyl benzene isomer	33±20
61	160	indan	112±53
62	161	indene	114±40
63	162	C_4-alkyl benzene isomer	T
64	164	C_4-alkyl benzene isomer	17±8
65	165	$C_{10}H_{20}$ isomer	10±2
66	165	$C_{10}H_{22}$ isomer	13±3
67	166	C_4-alkyl benzene isomer	T
68	167	$C_{10}H_{20}$ isomer	T
69	168	C_4-alkyl benzene isomer	T
70	168	$C_{10}H_{22}$ isomer	82±44
71	168	C_4-alkyl benzene isomer	
72	168	C_4H_7-benzene isomer	
73	170	C_4H_9-benzene isomer	T
74	170	C_4H_7-benzene isomer	T
75	171	$C_{11}H_{22}$ isomer	73±60
76	171	methylbenzofuran isomer	127±50
77	172	$C_{11}H_{24}$ isomer	177±37
78	173	C_5H_9-benzene isomer	367±74
79	176	C_4H -benzene isomer	T
80	179	methylindan isomer	19±7.4
81	180	C_5H_9-benzene isomer	37±6
82	180	$C_{11}H_{22}$ isomer	
83	180	methylindan isomer	39±19
84	181	methylindene isomer	57±37
85	182	methylindan isomer	24±20
86	183	C_5H_9-benzene isomer	80±37
87	184	methylindene isomer	55±37
88	184	ethylphenol isomer	NQ
89	185	C_5-alkyl benzene isomer	T
90	186	C_5-alkyl benzene isomer	T
91	187	$C_{11}H_{24}$ isomer	T
92	188	naphthalene	817±445
93	189	dimethylindan isomer	47±24
94	189	C_5-alkyl benzene isomer	84±23
95	189	$C_{12}H_{24}$ isomer	96±35
96	190	$C_{12}H_{26}$ isomer	74±34
97	190	dimethylindan isomer	82±44
98	191	C_6H_{13}-benzene isomer	T
99	192	dimethylbenzimidazole (tent.)	35±11

(continued)

Table C6 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb	Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
100	193	C_6H_7-benzene isomer	38±11			
101	196	C_6H_{13}-benzene isomer				
102	196	C_6H_{13}-benzene isomer				
103	196	dimethylindan isomer				
104	196	C_6H_{13}-benzene isomer	T			
105	199	C_4H_7-benzene isomer	6.7±3.3			
106	200	C_5H_9-benzene isomer	T			
107	200	C_6H_{13}-benzene isomer	3.3±2.0			
108	201	dimethylindole (tent.)	32±31			
109	201	$C_{11}H_{14}$ isomer	17±7			
110	202	C_7H_{15}-benzene isomer	3.3±2.0			
111	203	C_6H_{13}-benzene isomer	T			
112	204	$C_{11}H_{14}$ isomer	17.3±6.7			
113	205	C_6H_{13}-benzene isomer	T			
114	206	β-methylnaphthalene	350±83			
115	206	$C_{13}H_{28}$ isomer	38±5			
116	207	C_6H_{13}-benzene isomer	T			
117	208	C_6H_{13}-benzene isomer	T			
118	208	C_7H_{15}-benzene isomer	T			
119	210	α-methylnaphthalene	143±67			
120	210	C_6H_{11}-benzene isomer	T			
121	211	C_6H_{11}-benzene isomer	10±4.7			
122	211	C_7H_{15}-benzene isomer				
123	211	C_7H_{13}-benzene isomer				
124	214	C_8H_{17}-benzene isomer	T			
125	216	$C_{13}H_{18}$ isomer	39±11			
126	217	$C_{14}H_{26}$ isomer				
127	219	$C_{13}H_{18}$ isomer	11±6			
128	220	$C_{14}H_{24}$ isomer				
129	221	$C_{14}H_{30}$ isomer				
130	224	$C_{15}H_{24}$ isomer	T			
131	225	C_8H_{17}-benzene isomer	T			
134	240	dibenzofuran	T			

Table C7. VOLATILE ORGANICS IN TAR (-3T) FROM KNOCK-OUT CHAMBER DURING LOW BTU GASIFICATION OF ROSEBUD COAL (MERC, ERDA)

Chromatographic Peak No.	Elution Temp. (°C)	Compound	ppm
1	51	CO_2	-
2A	54	1-butene	NQ
2B	55	*n*-butane	NQ
4A	58	acetaldehyde	T
4B	60	furan	T
4C	60	*n*-pentane	4±2
5	61	propanal + propenal	T
5A	62	diethyl ether	2.8±1
6A	64	C_4H_8O isomer + acetone	T
6B	68	C_6H_{12} isomer	T
6C	69	C_6H_{14} isomer	T
7	71	hexafluorobenzene (eS)	
8	72	*n*-hexane	400±200
10	77	perfluorotoluene (eS)	
10A	77	methylcyclopentane	T
12	82	benzene	29±7.6
12A	88	C_7H_{16} isomer	T
12B	89	C_7H_{16} isomer	T
12C	89	$C_5H_{10}O$ isomer	T
12D	90	*n*-heptane	2±1
13	102	toluene	T
14	108	$C_6H_{12}O$ isomer	T
14A	110	*n*-octane	T
15B	121	ethylbenzene	T
16	123	*p*-xylene	22±6
16A	126	3-heptanone	T
16B	127	styrene	T
16C	127	2-heptanone	T
17	128	*o*-xylene	5±3
17A	129	*n*-heptanal	T
17B	130	C_9H_{18} isomer	T
18	131	*n*-nonane	10±6
18A	133	C_9H_{18} isomer	T
18B	134	$C_{10}H_{22}$ isomer	T
18C	135	isopropylbenzene + $C_{10}H_{22}$ isomer	T
18D	138	$C_8H_{16}O$ isomer	T
18E	138	$C_{10}H_{20}$ isomer	T
18F	139	$C_{10}H_{22}$ isomer	T
18G	141	$C_{10}H_{22}$ isomer	T
19	142	*n*-propylbenzene	T
19A	143	benzaldehyde	29±14
20	144	*p*-ethyltoluene	20±10
21	146	1,3,5-trimethylbenzene	24±6
21A	147	C_3-alkyl thiophene isomer	T
22	148	$C_{10}H_{22}$ isomer	T
23	150	*o*-ethyltoluene	20±8
23A	151	$C_{10}H_{20}$ + C_3-alkyl thiophene isomers	20±5
23B	151	2-octanone	T
23c	152	$C_{10}H_{20}$ isomer	T
23D	152	α-methylstyrene	40±10
24	153	1,2,4-trimethylbenzene	64±32
24A	153	$C_{10}H_{18}$ + $C_{10}H_{20}$ isomers	11±3
26	155	*n*-decane	60±20
26A	155	$C_{10}H_{20}$ isomer	31±4.2
26B	156	C_3-alkyl thiophene isomer	T
26C	157	$C_{10}H_{20}$ isomer	T
26D	158	C_4-alkyl benzene isomer	56±28
27	158	1,2,3-trimethylbenzene	T
27A	159	C_4-alkyl benzene isomer	T
27B	159	$C_{11}H_{24}$ isomer	T
28	161	indan	69±30
28A	161	C_4-alkyl benzene isomer	T
29	162	indene	120±40
29A	163	$C_{11}H_{22}$ isomer	T
30	163	C_4-alkyl benzene isomer	T
31	164	*n*-butylbenzene + *m*-diethylbenzene	48±29
31A	165	C_4-alkyl thiophene isomer	T
32	166	$C_9H_{18}O$ + $C_{11}H_{24}$ isomers + acetophenone	660±154
33	167	propyltoluene isomer	T
33A	167	$C_{11}H_{24}$ isomer	T
33B	168	$C_{10}H_{12}$ + $C_{11}H_{22}$ isomer	T
34	168	C_4-alkyl benzene isomer	T
35	169	2-nonanone + $C_{10}H_{12}$ isomer	60±20
36	170	C_4-alkyl benzene isomer	T
36A	170	$C_{10}H_{12}$ isomer	T
37	171	$C_{11}H_{22}$ isomer	6±2
37A	172	methylbenzimidazole isomer	60±10
37B	173	C_5-alkyl benzene isomer	T
38	173	*n*-undecane	320±100
38A	174	C_4-alkyl benzene isomer	T
39	174	methylbenzofuran isomer	186±123
39A	175	C_5-alkyl benzene isomer	T
39B	175	$C_{11}H_{22}$ isomer	T
39C	176	$C_{11}H_{14}$ isomer	T
40	176	C_4-alkyl benzene isomer	T
40A	177	$C_{11}H_{14}$ isomer	T
40B	178	$C_{12}H_{26}$ isomer	T
41	179	C_5-alkyl benzene isomer	9±3

(continued)

Table C7 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppm
41A	179	$C_{11}H_{12}$ isomer	3±1
42	180	methylindan isomer	75±15
42A	180	C_5-alkyl benzene isomer	T
42B	181	$C_{11}H_{22}$ isomer	T
43	181	methylindene isomer	400±17.5
43A	182	methylindan isomer	114±50
43B	182	C_4-alkyl benzene isomer + *n*-pentylbenzene	57±29
44	183	methylindene isomer	365±170
44A	184	C_5-alkyl benzene + $C_{12}H_{24}$ isomers	40±10
45	185	C_5-alkyl benzene isomer	44±8
45A	186	$C_{12}H_{26}$ isomer	220±160
46	187	C_5-alkyl benzene isomer	T
46A	188	C_2-alkyl indan isomer + 3-decanone	22±11
46B	188	2-decanone	T
47	189	naphthalene	7250±1810
47A	190	$C_{12}H_{24}$ isomer	T
47B	190	$C_{11}H_{14}$ isomer	T
47C	191	benzothiophene	301±200
47D	191	C_2-alkyl indan + C_5 alkyl benzene isomers	150±30
48	192	*n*-dodecane	560±60
48A	192	dimethylbenzofuran isomer	657±300
48A	193	C_6-alkyl benzene isomer	T
49	194	dimethylbenzofuran isomer	375±165
49A	194	$C_{13}H_{28}$ isomer	T
50	195	dimethylbenzimidazole isomer	571±280
50A	195	C_6-alkyl benzene isomer	T
50B	196	$C_{13}H_{26}$ isomer	T
50C	197	C_3-alkyl indan isomer	T
51	197	C_2-alkyl indan + C_6-alkyl benzene isomers	T
51A	198	C_3-alkyl indan + $C_{13}H_{24}$ isomers	T
51B	198	$C_{13}H_{26}$ + C_6-alkyl benzene isomers	T
51C	199	$C_{11}H_{12}$ isomer	2±1
52	199	$C_{13}H_{26}$ isomer	T
52A	200	$C_{11}H_{12}$ + C_3-alkyl indan isomers	11.6±2.8
53	200	C_2-alkyl indan isomer	14±3.6
54	201	phenyl-*n*-hexane	80±40
55	202	methyldihydronaphthalene isomer	160±40
55A	202	C_6-alkyl benzene isomer	22±7.6
55B	203	$C_{13}H_{28}$ + C_2-alkyl indan isomers	65±10
56	204	$C_{14}H_{30}$ isomer	44±5
56A	204	$C_{12}H_{16}$ isomer	T
56B	205	$C_{13}H_{24}$ isomer	T
56C	205	$C_{13}H_{26}$ + $C_{11}H_{14}$ isomers	T
57	206	$C_{13}H_{26}$ isomer	39±3.4
57A	207	$C_{14}H_{28}$ isomer	T
58	207	β-methylnaphthalene	114±46
59	208	*n*-tridecane	704±60
59A	209	$C_{14}H_{28}$ isomer	340±100
60	210	$C_{13}H_{26}$ isomer + α-methylnaphthalene	53±27
60A	210	C_3-alkyl indan isomer	T
61	211	$C_{14}H_{30}$ isomer	T
62	212	$C_{12}H_{16}$ + $C_{14}H_{28}$ isomer	T
63	214	$C_{14}H_{28}$ isomer	T
63A	215	$C_{15}H_{30}$ + $C_{15}H_{12}$ isomer	10±5
64	215	$C_{13}H_{26}$ isomer	T
65	216	$C_{15}H_{30}$ isomer	T
66	217	$C_{14}H_{30}$ isomer	T
67	218	$C_{14}H_{28}$ isomer	T
68	219	$C_{15}H_{32}$ isomer	20±10
69	221	$C_{14}H_{28}$ isomer	T
70	222	*n*-tetradecane	56±28
71	224	$C_{15}H_{30}$ isomer	T
71B	227	$C_{15}H_{32}$ isomer	T
71C	233	$C_{15}H_{30}$ isomer	T
71D	236	*n*-pentadecane	11±3

Table C8. VOLATILE ORGANICS IN AQUEOUS CONDENSATE (-4L) FROM LOW BTU GASIFICATION OF ROSEBUD COAL (MERC, ERDA)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
1	51	CO_2	-
1B	55	1-butane	NQ
1C	55	*n*-butane	T
1D	56	2-butene	T
3	60	acetaldehyde	92±53
3A	60	furan + *n*-pentane	7±4.3
3B	61	propanal + propenal	8.3±4.0
4	62	acetone	259±50
4B	67	butanal (tent.)	42±33
5	71	hexafluorobenzene (eS)	
5A	72	methyl ethyl ketone	22±8.3
6	75	perfluorotoluene (eS)	
7	80	benzene	1214±325
7A	81	thiophene	59±5.7
7B	85	cyclohexane	5.7±3.7
8	86	2-pentanone	12.3±5
8A	88	3-pentanone	T
9	89	$C_6H_{12}O$ isomer (tent.)	18±3.3
10	96	4-methyl-2-pentanone	78±33
10A	97	2-methyl-3-pentanone	93±42
11	99	3-methyl-2-pentanone	446±222
12	101	toluene	121±44
12A	101	2-methylthiophene	134±17
12B	103	3-methylthiophene	107±23
13	104	3-hexanone	86±37
14	105	2-hexanone	202±67
14A	107	3-methylpentanal (tent.)	185±42
14B	109	C_7H_{14} isomer	T
14C	110	*n*-octane	11±5
15A	116	diisopropyl ketone	T
15B	117	$C_7H_{14}O$ isomer	T
15C	118	$C_7H_{12}O$ isomer	T
16	119	$C_8H_{16}O$ isomer	T
17	121	ethylbenzene	104±42
17A	122	ethylthiophene isomer	83±42
17B	122	dimethylthiophene isomer	14±3.3
18	123	*p*-xylene	61±25
18A	124	dimethylthiophene isomer	28±3.3
19	125	3-heptanone	67±33
20	126	2-heptanone	195±50
20A	127	styrene	83±48
21	128	*o*-xylene	181±17
21A	129	C_9H_{18} isomer	T
21B	130	dimethylthiophene isomer	14±2.6
22	131	*n*-nonane	42±25
22A	132	anisole	5±2
22B	133	C_9H_{18} isomer	T
23	135	isopropylbenzene	26±5
23A	135	$C_{10}H_{22}$ isomer	T
23B	136	4-methyl-3-heptanone	T
24	137	2-methyl-3-heptanone	13±3.3
25	139	3-methyl-2-heptanone + α-methylstyrene	4.3±2
25A	140	octanone isomer	T
26	141	*n*-propylbenzene	T
26A	142	benzaldehyde + C_3-alkyl thiophene isomer	T
27	143	*m*-ethyltoluene	278±5.6
28	144	1,3,5-trimethylbenzene	139±17
28A	145	$C_{10}H_{22}$ isomer	T
28B	146	C_3-alkyl thiophene isomer	T
28C	146	$C_{10}H_{20}$ isomer	T
29	147	*o*-ethyltoluene	148±17
29A	148	C_3-alkyl thiophene isomer	20±5
30	150	2-octanone	188±100
30A	150	$C_{10}H_{16}$ isomer	T
30B	151	benzofuran	267±67
31	152	1,2,4-trimethylbenzene + $C_{10}H_{20}$ isomer	198±100
32	154	*n*-decane	134±43
32A	155	$C_{10}H_{20}$ isomer	T
32B	155	C_3-alkyl thiophene isomer + phenol	NQ
32C	156	C_4-alkyl benzene isomer	T
32D	157	ter-butyl benzene	T
33	158	1,2,3-trimethylbenzene	361±200
34	160	indan	247±47
35	162	indene	363±75
36	163	sec-butylbenzene	83±17
36A	164	C_4-alkyl benzene isomer	T
37	164	isobutylbenzene + C_4-alkyl thiophene isomer	95±33
37A	165	C_4-alkyl thiophene isomer	T
38	165	$C_9H_{18}O$ isomer	T
39	166	*p*-propyltoluene	99±50
39A	167	C_4-alkyl thiophene isomer	T
39B	167	methylindan isomer	T
40	168	C_4-alkyl benzene isomer + 3-nonanone	T
41	169	2-nonanone	156±83
42	169	C_4-alkyl benzene isomer	T
43	170	methylindan isomer	52±19

(continued)

Table C8 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
43A	171	$C_{11}H_{22}$ + C_4-alkyl benzene isomers	T
44	171	2-methylbenzimidazole	58±16
44A	172	C_5-alkyl benzene isomer	T
45	173	*n*-undecane	259±59
46	174	2-methylbenzofuran	391±20
46A	174	C_5-alkyl benzene isomer	T
47	175	$C_{11}H_{22}$ + methylbenzofuran isomers	60±20
48	176	tetramethylbenzene isomer	T
49	177	$C_{12}H_{26}$ isomer	T
50	177	$C_{11}H_{14}$ + $C_{12}H_{16}$ isomers	T
51	179	C_5-alkyl benzene isomer	T
51A	179	$C_{12}H_{16}$ isomer	T
52	180	$C_{11}H_{14}$ isomer	T
52A	181	C_5-alkyl benzene isomer	T
52B	181	methylindene isomer	222±40
53	182	methylindan isomer	90±43
53A	183	pentylbenzene	60±20
54	184	methylindene isomer	209±78
54A	185	C_5-alkyl benzene isomer	T
55	185	C_5-alkyl benzene isomer	8±1.7
55A	186	C_5-alkyl benzene isomer	T
56	187	3-decanone	139±67
56A	187	dimethylindan isomer	T
57	188	2-decanone	T
58	189	naphthalene	5121±1336
58A	189	dimethylindan isomer	T
58B	190	benzothiophene	52±20
58C	191	dimethylindan isomer	T
59	191	*n*-dodecane	297±74
60	193	5,6-dimethylbenzimidazole	T
60A	194	$C_{13}H_{28}$ isomer	T
60B	194	C_3-alkyl indan isomer	20±3
61	195	C_6-alkyl benzene isomer	40±2
62	197	$C_{11}H_{14}$ isomer	T
62A	198	C_6-alkyl benzene isomer	T
62B	198	$C_{12}H_{16}$ + methyldihydronaphthalene isomers	18±3
63	199	C_6-alkyl benzene + $C_{12}H_{24}$ isomers	T
64	200	$C_{11}H_{14}$ isomer	26±11
64A	200	C_6-alkyl benzene isomer	T
65	201	hexylbenzene	18±5
65A	201	6-methyl-1,2-dihydronaphthalene	42±16
66	202	C_6-alkyl benzene isomer	2.6±1
66A	202	C_3-alkyl indan isomer	T
67	203	methyldihydronaphthalene isomer	118±50
68	204	2-undecanone + $C_{12}H_{16}$ isomer	65±33
69	205	$C_{13}H_{26}$ isomer	3.3±1.7
69A	205	$C_{12}H_{16}$ isomer	T
70	206	*n*-tridecane + β-methylnaphthalene	967±225
71	208	$C_{12}H_{16}$ isomer	T
72	209	α-methylnaphthalene	278±26
73	210	$C_{12}H_{16}$ isomer	T
74	211	$C_{13}H_{18}$ + C_7-alkyl benzene isomers	T
75	212	C_7-alkyl benzene isomer	T
75A	213	$C_{13}H_{18}$ isomer	T
76	214	$C_{14}H_{28}$ isomer	T
76A	215	$C_{15}H_{32}$ isomer	T
77	216	phenylheptane	25±5
77A	216	C_4-alkyl indan isomer	T
78	217	C_7-alkyl benzene isomer	T
78A	217	$C_{15}H_{14}$ isomer	T
79	218	$C_{15}H_{32}$ isomer	5.6±1
80	220	$C_{14}H_{28}$ isomer	5.3±1
81	221	*n*-tetradecane	185±45
82	223	$C_{15}H_{32}$ isomer	74±44
82A	224	dimethylnaphthalene isomer	12±3.3
83	226	dimethylnaphthalene isomer	24±5
83A	229	dimethylnaphthalene isomer	9±3.3
83B	240	trimethylnaphthalene isomer	5±3
83C	240	trimethylnaphthalene isomer	11±3.7
83D	240	C_3-alkyl naphthalene isomer	2.6±0.6

Table C9. VOLATILE ORGANICS IN TAR (-5T) FROM KNOCK-OUT CHAMBER DURING LOW BTU GASIFICATION OF ROSEBUD COAL (MERC, ERDA)

Chromatographic Peak No.	Elution Temp. (°C)	Compound	ppm
1	50	CO_2	-
2A	53	1-butene	NQ
2B	54	*n*-butane	NQ
2C	57	C_5H_{10} isomer	T
3	58	acetaldehyde	29±10
3A	59	furan	T
3B	60	*n*-pentane	7±3.5
4	60	propanal + propenal	T
4A	62	diethyl ether	T
5A	63	acetone	T
5B	69	C_6H_{14} isomer	T
6	71	hexafluorobenzene (e*)	
7	72	*n*-hexane	4.2±2
9	76	perfluorotoluene (e*)	
9A	77	methylcyclopentane	3.8±0.6
9C	81	benzene	21±3
9D	83	C_7H_{16} isomer	T
9E	85	C_7H_{16} isomer	T
9G	88	C_7H_{16} isomer	T
9H	89	$C_5H_{10}O$ isomer (tent.)	T
9I	90	C_7H_{16} isomer	T
10	102	toluene	415±207
11	109	$C_6H_{12}O$ isomer	11±2.4
12	110	*n*-octane	T
14A	119	furfural (tent.)	T
14B	121	ethylbenzene	5.6±0.6
14C	123	*p*-xylene	10±1
14D	127	styrene	T
14E	128	2-heptanone	T
15	128	*o*-xylene	13±3.4
15A	129	C_9H_{18} isomer	T
16	131	*n*-nonane	38±3
16A	135	$C_8H_{16}O$ isomer + isopropylbenzene	T
16B	136	$C_{10}H_{22}$ isomer	T
16C	139	$C_{10}H_{22}$ isomer	T
16D	143	*n*-propylbenzene	T
16E	144	benzaldehyde	14.2±6.4
17	145	*m*-ethyltoluene	T
17A	146	C_3-alkyl thiophene isomer	T
17B	147	1,3,5-trimethylbenzene	T
18	148	$C_{10}H_{22}$ isomer	T
19	149	*o*-ethyltoluene	7.2±3.6
19A	150	2-octanone	T
19B	151	$C_{10}H_{20}$ isomer	T
19C	151	α-methylstyrene	29±12
20	152	1,2,4-trimethylbenzene	21.4±10
22	154	*n*-decane	T
22A	155	$C_{10}H_{20}$ isomer	T
22B	156	phenol	NQ
22C	156	$C_{10}H_{20}$ isomer	T
23	157	1,2,3-trimethylbenzene	62.8±20
23A	158	C_4-alkyl benzene isomer	11.8±3.8
24	160	indan	30±4
24A	160	C_4-alkyl benzene isomer	15±2.4
25	161	indene	57.2±28
25A	162	C_4-alkyl benzene isomer	T
26	162	C_4-alkyl benzene isomer	12.4±3
26A	163	C_4-alkyl benzene isomer	3.4±2.2
27	164	sec-butylbenzene	T
27A	164	C_4-alkyl thiophene isomer	1±0.6
28	165	acetophenone	T
29	166	C_4-alkyl benzene isomer	11±3.4
29A	166	C_4-alkyl thiophene isomer	13.2±3.6
29B	167	$C_{10}H_{12}$ isomer	10±5
30	168	C_4-alkyl benzene isomer	15.8±3.8
30A	168	2-nonanone	30.6±14
31	169	C_4-alkyl benzene isomer	T
31A	169	$C_{10}H_{12}$ isomer	T
32	170	$C_{11}H_{22}$ + C_4-alkyl benzene isomers	T
32A	171	methylbenzimidazole isomer	14.2±7.2
32B	171	$C_{11}H_{22}$ isomer	T
32C	172	C_5-alkyl benzene isomer	T
33	172	*n*-undecane	160±40
34	173	methylbenzofuran isomer	91±44
34A	173	C_4-alkyl benzene isomer	T
34B	174	C_5-alkyl benzene isomer	T
34C	174	$C_{11}H_{22}$ isomer	T
35	175	tetramethylbenzene isomer	T
35A	175	$C_{12}H_{26}$ isomer	T
36	176	$C_{10}H_{12}$ isomer	T
36A	177	$C_{11}H_{14}$ isomer	T
37	178	C_5-alkyl benzene isomer	T
37A	178	C_5-alkyl benzene isomer	T
38	179	$C_{10}H_{12}$ isomer	T
38A	179	C_5-alkyl benzene isomer	T
39	180	C_5-alkyl benzene isomer	T
40	181	methylindene isomer	152±70
40A	181	methylindan + C_5-alkyl benzene isomers	76±28
41	182	methylindene isomer	157±64

(continued)

Table C9 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppm
41A	182	C_5-alkyl benzene isomer	23±3.4
41B	183	$C_{12}H_{26}$ + $C_{10}H_{20}O$ isomer	16±4
42	183	C_5-alkyl benzene isomer	15.6±2
42A	185	C_5-alkyl benzene isomer	11±3
43	185	$C_{12}H_{26}$ isomer	T
43A	186	dimethylindan isomer	T
44	186	2-decanone	57±29
45	187	naphthalene	2890±500
45A	188	C_2-alkyl indan + $C_{12}H_{24}$ isomers	T
45B	188	benzothiophene	61±25
46	189	C_2-alkyl indan isomer + n-dodecane	390±140
46A	190	dimethylbenzofuran isomer	152±65
46B	191	C_6-alkyl benzene + $C_{12}H_{24}$ isomers	T
46C	192	dimethylbenzofuran isomer	202±40
47	192	$C_{13}H_{28}$ isomer	T
48	193	C_6-alkyl benzene isomer	T
48A	194	C_3-alkyl indan isomer	T
48B	195	$C_{13}H_{26}$ + C_2-alkyl indan isomers	T
49	195	C_6-alkyl benzene isomer	T
49A	196	C_3-alkyl indan isomer	T
49B	196	C_6-alkyl benzene isomer	T
50	197	$C_{13}H_{26}$ + C_6-alkyl benzene isomers	T
50A	198	$C_{12}H_{14}$ isomer	T
51	199	phenyl-n-hexane	28.6±14
52	200	methyldihydronaphthalene + $C_{13}H_{28}$ + C_6-alkyl benzene isomers	143±45
53	201	methyldihydronaphthalene isomer	171±62
54	202	$C_{14}H_{30}$ + C_7-alkyl benzene isomer	T
54A	202	C_3-alkyl indan isomer	T
55	203	2-undecanone	3.6±3.2
56	204	$C_{12}H_{16}$ isomer	40±10
57	205	$C_{13}H_{26}$ isomer	78±22
57A	205	C_3-alkyl indan + $C_{14}H_{28}$ isomers	40±10
58	206	n-tridecane + β-methylnaphthalene	1267± 240
59	208	$C_{12}H_{16}$ isomer	T
59A	209	C_7-alkyl benzene isomer	T
60	210	α-methylnaphthalene	714±240
61	211	$C_{12}H_{16}$ isomer	T
61A	212	C_7-alkyl benzene isomer	T
62	212	C_4-alkyl indan isomer	T
62A	213	$C_{14}H_{28}$ isomer	T
63	214	$C_{12}H_{16}$ + $C_{13}H_{18}$ + $C_{13}H_{26}$ isomers	19.8±3.8
63A	214	$C_{15}H_{30}$ isomer	T
63B	215	$C_{12}H_{14}$ isomer	T
64	215	phenyl-n-heptane	42.8±15
64A	216	C_4-alkyl indan isomer	11.2±2
65	216	$C_{15}H_{14}$ + C_7-alkyl benzene isomers	15±5
65A	217	C_4-alkyl indan isomer	20±10
65B	217	$C_{14}H_{28}$ isomer	20±5
66	218	$C_{15}H_{32}$ isomer	22.4
67	219	$C_{14}H_{28}$ isomer	235±3
67A	220	$C_{15}H_{12}$ isomer	40±10
67B	220	$C_{13}H_{18}$ isomer	35±15
68	221	n-tetradecane	T
68A	222	$C_{13}H_{18}$ isomer	T
69	223	$C_{14}H_{28}$ isomer	T
69A	223	$C_{15}H_{30}$ isomer	T
69B	224	C_8-alkyl benzene isomer	T
69C	225	C_5-alkyl indan or $C_{14}H_{20}$ isomer	T
69D	226	$C_{16}H_{32}$ isomer	T
69E	227	$C_{15}H_{30}$ isomer	T
69F	227	C_8-alkyl benzene isomer	T
70	228	C_9-alkyl benzene + $C_{16}C_{32}$ isomers	T
71	229	$C_{16}H_{32}$ isomer	60±22
73	234	$C_{15}H_{30}$ isomer	51±12
74	236	n-pentadecane	77±29

Table C10. VOLATILE ORGANICS IN AQUEOUS CONDENSATE (-6L) FROM LOW BTU GASIFICATION OF ROSEBUD COAL (MERC, ERDA)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
1	50	CO_2	-
2A	53	1-butene	NQ
2B	54	*n*-butane	NQ
3A	58	acetaldehyde + C_5H_{10} isomer	
3B	58	furan	T
3C	59	propanal + propenal	16±2.3
3D	59	*n*-pentane + C_5H_{10} isomer	167±50
4	60	acetone	20±4.3
5A	66	butanal	T
5B	67	butenal isomer (tent.)	T
5C	68	C_6H_{14} isomer	5±2.3
5D	69	propionitrile	T
6	70	hexafluorobenzene (eS)	
6A	70	*n*-hexane	100±50
7	71	methyl ethyl ketone	92±18
9	74	C_6H_{12} isomer	T
10	75	perfluorotoluene (eS)	
10A	76	methylcyclopentane	27±21
11	80	benzene	1457±170
11A	81	thiophene	45±57
11B	82	methyl isopropyl ketone	T
12	86	2-pentanone	260±79
12A	88	3-pentanone	10±5
12B	89	C_7H_{16} isomer	18±6
12C	90	2-methylbutanal (tent.)	9±7
12D	93	pentanal (tent.)	T
12E	94	C_7H_{12} isomer	T
12F	95	dimethyl disulfide	T
12G	96	4-methyl-2-pentanone	17±5
12H	98	2-methyl-3-pentanone	83±33
12I	99	3-methyl-2-pentanone	33±17
13	101	toluene	
13A	103	2-methylthiophene	9±5
13B	105	3-hexanone	117±44
14	106	2-hexanone	75±40
14A	107	3-methylpentanal (tent.)	209±83
14B	108	*n*-hexanal (tent.)	T
14C	109	*n*-octane	6.7±3.4
14D	110	C_8H_{16} isomer	T
16A	115	5-methyl-3-hexanone	29±15
16B	116	2-methyl-3-hexanone	32±17
16C	117	C_9H_{20} isomer	T
17	118	$C_8H_{16}O$ isomer (tent.)	T
17A	120	$C_7H_{14}O$ isomer	T
18	121	ethylbenzene	160±40
18A	122	ethylthiophene isomer	19±14
18B	122	dimethylthiophene isomer	24±19
19	123	*p*-xylene	481±226
20	124	dimethylthiophene isomer	64±30
21	126	3-heptanone	80±44
22	127	2-heptanone	148±25
22A	127	styrene	44±25
23	128	*o*-xylene	312±100
23A	129	C_9H_{18} isomer	T
23B	130	dimethylthiophene isomer	11±11
24	131	*n*-nonane	17±5.3
24A	132	anisole	T
24B	135	isopropylbenzene	15±7.3
24C	136	4-methyl-3-heptanone	T
25	137	2-methyl-3-heptanone	T
25A	138	$C_{10}H_{20}$ isomer	T
25B	139	3-methyl-2-heptanone + α-methylstyrene	T
25C	140	6-methyl-2-heptanone	16.7±8.3
25D	141	5-methyl-2-heptanone	8.3±4.3
26	142	*n*-propylbenzene	T
26A	143	benzaldehyde	67±34
26B	143	C_3-alkyl thiophene isomer	4±2
27	144	*p* or methyltoluene	189±75
28	146	1,3,5-trimethylbenzene	66±33
28A	147	$C_{10}H_{22}$ + C_3-alkyl thiophene isomers	19±19
29	148	*o*-ethyltoluene	134±66
29A	148	3-octanone	47±23
29B	149	C_3-alkyl thiophene isomer	5.7±3.7
30	149	2-octanone	150±67
31	151	benzofuran	267±66
31A	151	1,2,4-trimethylbenzene	234±83
33	153	*n*-decane	30±15
33A	154	$C_{10}H_{20}$ isomer	T
33B	154	C_3-alkyl thiophene isomer	T
33C	155	phenol	NQ
33D	156	C_4-alkyl benzene + $C_9H_{18}O$ isomers	T
34	157	1,2,3-trimethylbenzene	267±100
34A	158	C_4-alkyl benzene isomer	17±67
34B	159	alkyl alcohol (tent.) + C_4-alkyl thiophene isomers	5.3±3.7
35	160	indan	200±100
36	161	indene	267±134
36A	162	sec-butylbenzene	33±16
37	163	isobutylbenzene + *o*-cymene	111±55

(continued)

Table C10 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
37A	164	C_4-alkyl thiophene isomer	T
38	164	acetophenone	10±5
38A	165	$C_9H_{18}O$ isomer	T
39	166	*p*-propyltoluene	16.7±10
39A	167	3-nonanone	T
40	167	*m*-propyltoluene	70±50
41	168	2-nonanone + C_4-alkyl benzene isomer	T
41A	169	$C_{10}H_{12}$ isomer	3.3±0.7
42	170	$C_{11}H_{22}$ isomer + 2-methyl-benzimidazole	T
42A	171	C_4-alkyl benzene isomer	T
43	172	*n*-undecane	40±20
44	173	2-methylbenzofuran	134±66
44A	174	C_5-alkyl benzene isomer	20±6
45	175	tetramethylbenzene isomer	T
45A	176	methylbenzofuran isomer	T
45B	177	$C_{10}H_{20}O$ isomer	T
45C	178	C_5-alkyl benzene + $C_{10}H_{20}O$ isomers	13±4.7
46	179	methylindan isomer	17±5.6
46A	180	C_5-alkyl benzene + dimethyl-phenol isomers	NQ
46B	180	$C_{12}H_{26}$ + methylindene isomers	83±42
47	181	methylindan isomer	T
47A	181	pentylbenzene	T
48	182	1-methyl-1H-indene	
48A	183	$C_{11}H_{14}$ isomer	T
49	183	C_5-alkyl benzene isomer	42±6.3
49A	184	$C_{12}H_{24}$ isomer	3.7±1
49B	184	dimethylphenol isomer	NQ
49C	185	3-decanone	T
50	186	2-decanone	T
51	187	naphthalene	3574±267
51A	188	benzothiophene	89±43
51B	189	dimethylindan isomer	T
52	189	*n*-dodecane	T
52A	190	$C_{10}H_{10}O$ isomer	T
52B	191	C_6-alkyl benzene isomer	1.7±0.3
53	191	dimethylbenzofuran isomer	134±78
53A	192	$C_{12}H_{16}$ isomer	1.7±0.7
54	193	$C_{11}H_{14}$ isomer	37±17
55	195	ethylindan + C_6-alkyl benzene isomers	42±17
55A	196	C_6-alkyl benzene isomer	T
55B	197	C_3-alkyl indan isomer	T
56	198	dimethylindan isomer	13±5.6
57	199	methyldihydronaphthalene isomer	35±9.7
58	200	C_2-alkyl indan isomer	15±6.7
58A	201	3-undecanone + $C_{11}H_{12}$ isomer	T
59	202	C_3-alkyl indan isomer + 2-undecanone	NQ
60	204	$C_{13}H_{26}$ isomer	24±12
60A	204	6-methylbenzo(b)thiophene	7±3.4
60B	205	C_3-alkyl indan + $C_{13}H_{26}$ isomers	5±1.7
60C	205	*n*-tridecane	T
61	206	β-methylnaphthalene	57±10
62	207	C_3-alkyl indan isomer	189±17
63	209	α-methylnaphthalene	50±10
64	210	$C_{12}H_{16}$ isomer	9.6±9
64A	212	C_7-alkyl benzene isomer	T
64B	213	C_4-alkyl indan isomer	T
65	213	$C_{12}H_{16}$ isomer	22±11
65A	214	C_7-alkyl benzene isomer	T
65B	214	C_4-alkyl indan isomer	T
65C	215	$C_{13}H_{18}$ + C_7-alkyl benzene isomers	T
66	218	biphenyl	67±16.7
66A	219	$C_{13}H_{18}$ isomer	T
67	221	*n*-tetradecane	3.3±0.7
67A	221	ethylnaphthalene isomer	T
67B	222	$C_{13}H_{18}$ isomer	T
68	223	dimethylnaphthalene isomer	T
68A	224	$C_{13}H_{18}$ isomer	T
69	226	dimethylnaphthalene isomer	T
69A	230	$C_{14}H_{20}$ isomer	T
69B	235	*n*-pentadecane	T

Table C11. VOLATILE ORGANICS IN TAR (-7T) FROM KNOCK-OUT CHAMBER DURING LOW BTU GASIFICATION OF ROSEBUD COAL (MERC, ERDA)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppm
1	50	CO_2	-
3	57	C_3H_8 isomer	NQ
5	59	C_4H_8 isomer	NQ
6	59	C_4H_{10} isomer	NQ
9	66	acetone	T
10	72	perfluorobenzene (eS)	
11	74	n-hexane	22
13	77	perfluorotoluene (eS)	
14	82	benzene	72.8
15	102	toluene	1334
16	108	C_7H_{12} isomer	T
17	111	C_7H_{16} isomer	T
19	127	ethylbenzene	T
20	128	p- and/or m-xylene	156
21	130	C_8H_{16} isomer	T
22	131	styrene and/or cyclooctatetraene	53.4
23	132	o-xylene	133
24	134	C_9H_{18} isomer	T
25	136	C_9H_{20} isomer	40
26	140	C_3-alkyl benzene isomer	T
27	141	$C_{10}H_{22}$ isomer	T
28	142	$C_{10}H_{22}$ isomer	T
29	143	$C_{10}H_{22}$ isomer	20
30	143	C_3-alkyl benzene isomer	24
31	146	C_3-alkyl benzene isomer	T
32	147	$C_{10}H_{22}$ isomer	29
33	147	C_3-alkyl benzene isomer	12
34	150	C_3-alkyl benzene isomer	T
35	151	$C_{10}H_{22}$ isomer	T
36	152	methylstyrene isomer	356
37	153	$C_{10}H_{20}$ isomer	45
38	153	C_3-alkyl benzene isomer	80
40	154	$C_{10}H_{22}$ isomer	200
41	155	$C_{10}H_{20}$ isomer	T
42	156	$C_{11}H_{22}$ isomer	T
43	157	C_4-alkyl benzene isomer	26
44	158	C_4-alkyl benzene isomer	250
45	158	$C_{11}H_{24}$ isomer	T
46	160	indan	244
47	162	C_4H_7-benzene isomer	T
48	162	indene	711
49	163	C_4-alkyl benzene isomer	T
50	163	$C_{11}H_{22}$ isomer	T
51	164	C_4-alkyl benzene isomer	124
52	165	$C_{11}H_{22}$ isomer	T
53	166	C_4-alkyl benzene isomer	T
54	166	$C_{11}H_{22}$ isomer	4
55	166	$C_{11}H_{20}$ isomer	T
56	167	C_4H_7-benzene isomer	T
57	167	$C_{11}H_{24}$ isomer	T
58	168	C_4-alkyl benzene isomer	T
59	168	$C_{10}H_{22}$ isomer	T
60	169	C_4-alkyl benzene isomer	88
61	169	C_4H_7-benzene isomer	60
62	171	C_4H_7-benzene isomer	10
63	171	$C_{11}H_{22}$ isomer	80
64	173	C_4H_7-benzene isomer	T
65	173	C_5-alkyl benzene isomer	T
66	173	$C_{11}H_{24}$ isomer	20
67	174	methylbenzofuran isomer	48
68	174	$C_{11}H_{22}$ isomer	190
69	175	dimethylindan isomer	1110
70	175	$C_{11}H_{22}$ isomer	T
71	176	C_5-alkyl benzene isomer	102
72	176	C_4H_7-benzene isomer	76
73	177	methylindan isomer	29
74	178	$C_{12}H_{26}$ isomer	T
75	179	C_5-alkyl benzene isomer	20
76	179	C_5H_9-benzene isomer	T
77	180	C_5-alkyl benzene isomer	76
78	180	$C_{12}H_{24}$ isomer	23
79	182	$C_{11}H_{22}$ isomer	T
80	183	C_5H_9-benzene isomer	T
81	183	$C_{12}H_{24}$ isomer	T
82	183	methylindene isomer	889
83	183	C_5-alkyl benzene isomer	280
84	184	C_5H_9-benzene isomer	40
85	185	$C_{12}H_{24}$ isomer	23
86	185	$C_{12}H_{26}$ isomer	T
87	186	$C_{13}H_{26}$ isomer	T
88	187	$C_{11}H_{24}$ isomer	T
89	189	naphthalene	50
90	189	C_6H_{11}-benzene isomer	T
91	189	$C_{12}H_{24}$ isomer	T
92	189	C_6H_{11}-benzene isomer	T
93	189	$C_{12}H_{26}$ isomer	T
94	189	C_5H_9-benzene isomer	T
95	189	C_6H_{11}-benzene isomer	T
96	190	C_5H_9-benzene isomer	T
97	190	C_6H_{11}-benzene isomer	T
98	190	$C_{12}H_{24}$ isomer	1040

(continued)

Table C11 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppm
99	190	$C_{12}H_{26}$ isomer	1860
100	190	$C_{13}H_{26}$ isomer	T
101	190	$C_{13}H_{28}$ isomer	T
102	191	C_6H_{13}-benzene isomer	50
103	191	C_6H_{11}-benzene isomer	T
104	193	$C_{13}H_{26}$ isomer	T
105	194	C_6H_{13}-benzene isomer	T
106	195	$C_{12}H_{24}$ isomer	T
107	195	C_7H_{15}-benzene isomer	70
108	196	C_5H_9-benzene isomer	T
109	197	naphthol	NQ
110	197	C_6H_{13}-benzene isomer	70
111	197	C_6H_{11}-benzene isomer	20
112	198	C_5H_7-benzene isomer	42
113	198	$C_{13}H_{28}$ isomer	65
114	199	$C_{14}H_{30}$ isomer	28
115	199	C_7H_{15}-benzene isomer	143
116	201	C_6H_{11}-benzene isomer	87
117	201	C_6H_{13}-benzene isomer	T
118	201	C_6H_9-benzene isomer	T
119	202	$C_{13}H_{26}$ isomer	T
120	203	C_6H_{11}-benzene isomer	T
121	206	$C_{14}H_{28}$ isomer	49
122	206	C_7H_{15}-benzene isomer	T
123	206	β-methylnaphthalene	2149
124	206	$C_{13}H_{28}$ isomer	1680
125	209	C_6H_{11}-benzene isomer	T
126	209	$C_{13}H_{26}$ isomer	T
127	209	$C_{14}H_{28}$ isomer	T
128	211	C_7H_{15}-benzene isomer	T
129	211	$C_{14}H_{30}$ isomer	56
130	213	α-methylnaphthalene	3160
131	213	C_7H_{13}-benzene isomer	T
132	214	C_7H_{15}-benzene isomer	1180
133	214	C_8H_{17}-benzene isomer	T
134	214	$C_{14}H_{24}$ isomer	T
135	214	C_7H_{13}-benzene isomer	T
136	214	$C_{15}H_{30}$ isomer	T
137	216	$C_{15}H_{28}$ isomer	40
138	216	C_7H_{15}-benzene isomer	38
139	217	$C_{14}H_{26}$ isomer	75
140	217	C_9H_{19}-benzene isomer	T
141	217	C_7H_{13}-benzene isomer	T
142	218	$C_{15}H_{32}$ isomer	1250
143	220	$C_{14}H_{28}$ isomer	62
144	220	C_7H_{13}-benzene isomer	T
145	222	C_7H_{13}-benzene isomer	T
146	222	$C_{14}H_{30}$ isomer	1070
147	222	C_9H_{19}-benzene isomer	T
148	222	$C_{15}H_{30}$ isomer	1860
149	222	$C_{15}H_{28}$ isomer	T
150	222	$C_{15}H_{26}$ isomer	T
151	223	$C_{14}H_{30}$ isomer	T
152	223	$C_{15}H_{30}$ isomer	T
153	224	C_2-alkyl naphthalene isomer	70
154	225	C_2-alkyl naphthalene isomer	56
155	225	C_7H_{13}-benzene isomer	T
156	226	C_8H_{17}-benzene isomer	T
157	227	C_9H_{19}-benzene isomer	T
158	228	$C_{15}H_{26}$ isomer	T
159	230	$C_{16}H_{32}$ isomer	T
160	230	$C_{16}H_{34}$ isomer	T
161	231	$C_{15}H_{26}$ isomer	1720
162	233	cyanophenol (tent.)	NQ
163	234	$C_{15}H_{32}$ isomer	102
164	236	$C_{15}H_{30}$ isomer	T
165	240	pentamethyldihydroindene	T
166	240	C_3-alkyl naphthalene isomer	T
167	240	C_3-alkyl naphthalene isomer	T
168	240	C_3-alkyl naphthalene isomer	T
169	240	fluorene	80
170	240	C_3-alkyl naphthalene isomer	T
171	240	C_3-alkyl naphthalene isomer	T

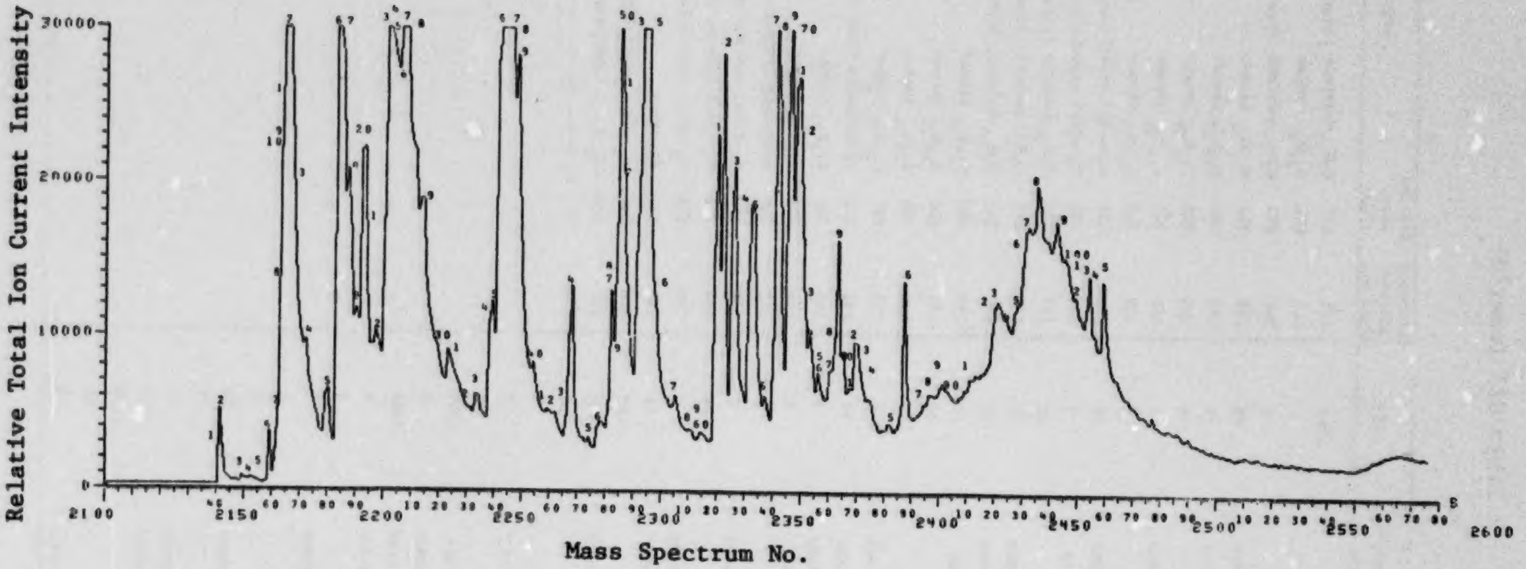


Figure C4. Profile of volatile organics in aqueous sample (-1L) from dewatering well #5 (LLL, ERDA).

Table C12. VOLATILE ORGANICS IN AQUEOUS SAMPLE (-1L) FROM DEWATERING WELL #5 (LLL, ERDA)

Chromatographic Peak No.	Elution Temp. (°C)	Compound	ppb
1	40	$N_2 + O_2$	-
2	41	CO_2	-
3	44	C_4H_8 isomer	NQ
4	45	C_4H_6 isomer	NQ
5	46	C_4H_8 isomer	NQ
7	51	C_5H_{12} isomer	T
9	51	C_4H_{10} isomer	T
10	51	ethanethiol	15.81±6.0
13	54	acetone	16.17±5.2
14	56	C_5H_8 isomer	1.50±0.8
15	60	methylbutanol (tent.)	2.60±1.2
16	63	perfluorobenzene (eS)	
17	63	C_6H_{14} isomer	9.87±4.6
19	65	methyl ethyl ketone (tent.)	10.59±7.25
20	67	C_6H_{12} isomer	3.75±1.8
21	68	perfluorotoluene (eS)	
23	71	C_6H_{10} isomer	6.26±2.4
24	71	benzene	192.51±3.3
25	72	thiophene	6.59±1.3
26	72	C_6H_{14} isomer	T
27	74	vinylcyclohexene (tent.)	0.41±0.4
29	74	dimethylfuran isomer	2.75±1.5
30	74	C_7H_{12} isomer	T
31	75	C_6H_{14} isomer	2.65±1.4
32	76	C_7H_{16} isomer	T
33	78	dimethyldisulfide	NQ
34	89	C_7H_{16} isomer	1.76±0.4
35	89	C_7H_{12} isomer	T
36	90	toluene	67.76±32
37	90	C_7H_{14} isomer	14.00+7.0
38	93	methylthiophene isomer	117.45±6.5
39	94	methylthiophene isomer	120.00±56
40	86	C_8H_{14} isomer	0.3±0.1
41	100	C_8H_{18} isomer	T
42	101	C_8H_{14} isomer	T
43	103	unknown	NQ
45	107	C_8H_{14} isomer	T
46	108	C_8H_{18} isomer	T
47	111	ethylbenzene	1.88±0.4
48	111	C_8H_{16} isomer	T
49	112	trimethylcyclohexene isomer	T
50	113	p- or m-xylene	4.70±1.3
51	114	C_8H_{16} isomer	1.34±0.8
52	114	C_2-alkyl thiophene isomer	1.30±0.6
53	116	C_2-alkyl thiophene isomer	1.25±0.7
54	117	styrene	3.80±1.2
55	117	o-xylene	6.47±1.5
56	119	C_2-alkyl thiophene isomer	8.00±2.5
57	123	anisole	0.59±0.4
58	125	C_9H_{20} isomer	T
59	127	C_9H_{18} isomer	T
60	127	C_9H_{20} isomer	T
61	130	C_3-alkyl benzene isomer	104.00±30
62	131	C_9H_{18} isomer	47.50±12
63	133	C_3-alkyl benzene isomer	5.98±1.3
64	135	benzofuran	4.89±2.0
66	139	C_3-alkyl thiophene isomer	3.50±1.2
67	141	C_4-alkyl benzene isomer	6.00±2.0
68	141	C_3-alkyl benzene isomer	8.35±2.5
69	143	methylstyrene isomer	1.06±0.4
70	143	$C_{10}H_{20}$ isomer	6.38±2.4
71	144	methylphenylacetylene	10.59±3.3
72	144	C_4-alkyl benzene isomer	0.50±0.2
73	145	$C_{10}H_{22}$ isomer	T
74	146	C_4-alkyl benzene isomer	0.25±0.2
75	147	$C_{10}H_{20}$ isomer	T
76	148	$C_{10}H_{20}$ isomer	1.46±0.6
77	150	C_4H_7-benzene isomer	0.65±0.3
78	151	C_4H_7-benzene isomer	0.68±0.2
79	151	C_4-alkyl benzene isomer	6.31±2.4
80	152	methylbenzofuran isomer	0.39±0.2
81	154	C_5-alkyl benzene isomer	0.10±0
82	155	C_4-alkyl benzene isomer	0.12±0
83	156	methylbenzofuran isomer	1.07±0.3
84	156	$C_{11}H_{22}$ isomer	T
85	160	C_5-alkyl benzene isomer	T
87	167	α-terpinene (tent.)	T
88	168	naphthalene	0.35±0.2
89	170	C_5H_9-benzene isomer	T
90	173	C_6-alkyl benzene isomer	T
91	175	C_6-alkyl benzene isomer	T
92	180	C_3-alkyl anisole isomer (tent.)	T
93	180	C_6H_{11}-benzene isomer	0.15±0
94	182	C_7-alkyl benzene isomer	0.17±0
95	183	quinoline	0.96±0.4
96	184	C_7-alkyl benzene isomer	T
98	187	C_6H_{11}-benzene isomer ?	NQ
100	191	C_4-alkyl phenol isomer	NQ
101	191	C_8-alkyl benzene isomer	0.05±0

(continued)

Table C12 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb	Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
102	192	C_7H_{13}-benzene isomer	T				
103	196	$C_{15}H_{30}$ isomer	1.44±0.7				
104	196	$C_{15}H_{32}$ isomer	0.50±0.3				
105	199	$C_{14}H_{30}$ isomer	2.10±0.6				

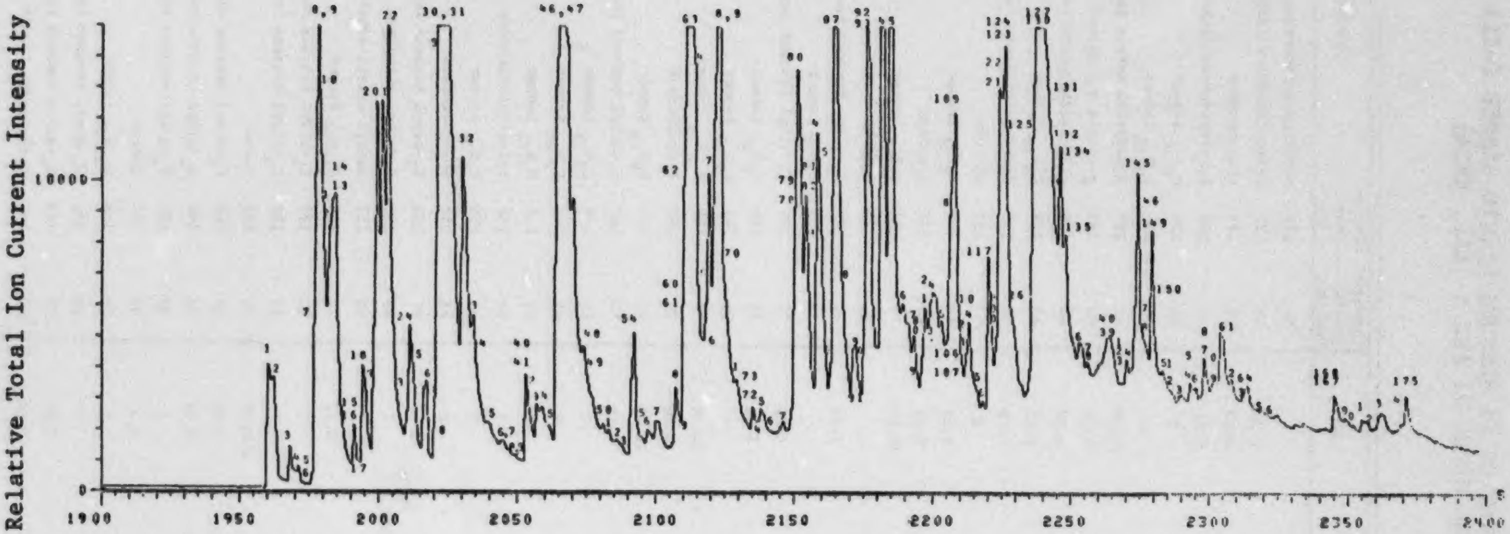


Figure C5. Profile of volatile organics in blended liquid sample (-2L) from dewatering wells #1 and 6 (LLL, ERDA).

Table C13. VOLATILE ORGANICS IN BLENDED LIQUID SAMPLE (-2L) FROM DEWATERING WELLS #1 AND 6 (LLL, ERDA)

Chromatographic Peak No.	Elution Temp. (°C)	Compound	ppb
1	52	CO_2	-
3	55	C_4H_8 isomer	0.35
4	55	C_4H_{10} isomer	0.10
5	56	C_4H_8 isomer	0.11
6	58	C_5H_{10} isomer	T
7	59	acetaldehyde	T
8	59	C_4H_{10} isomer	24.00
11	61	C_5H_{10} isomer	0.14
12	62	ethanethiol	4.20
13	63	acetone	0.25
16	66	cyclopentene	0.36
17	67	C_5H_{10} isomer	T
18	68	C_6H_{14} isomer	2.15
19	70	C_6H_{14} isomer	0.55
20	70	methyl ethyl ketone	14.00
21	71	perfluorobenzene (eS)	
22	72	C_6H_{14} isomer	7.15
24	76	perfluorotoluene (eS)	
25	77	methylcyclopentane	0.10
27	79	C_7H_{14} isomer	1.45
28	81	C_6H_{10} isomer	T
29	81	benzene	34.09
30	82	C_6H_{14} isomer	4.20
31	83	thiophene	12.75
32	86	C_6H_{14} isomer	4.20
34	89	C_6H_{14} isomer	T
35	90	dimethylfuran isomer	T
36	91	C_7H_{16} isomer	T
37	92	C_7H_{12} isomer	T
38	93	C_7H_{12} isomer	T
39	93	C_7H_{14} isomer	T
40	98	C_7H_{16} isomer	0.45
41	98	dimethyl disulfide (tent.)	T
42	99	C_7H_{12} isomer	T
43	99	C_7H_{16} isomer	0.17
44	99	C_7H_{16} isomer	T
45	100	C_7H_{12} isomer	T
46	103	toluene	150.00
47	104	methylthiophene isomer	2.98
48	106	methylthiophene isomer	2.25
49	106	C_7H_{16} isomer	T
50	107	C_7H_{16} isomer	0.32
51	108	C_8H_{14} isomer	T
52	111	trimethylfuran isomer	T
53	112	C_8H_{14} isomer	0.05
55	118	C_8H_{18} isomer	0.04
56	119	methylcyclopentanone isomer	0.14
57	121	thiacyclohexane (tent.)	0.22
58	124	ethylbenzene	0.46
59	125	ethylthiophene isomer	0.11
60	126	C_8H_{16} isomer	17.00
61	126	C_9H_{16} isomer	19.25
62	127	dimethylthiophene isomer	0.40
63	127	p-xylene + m-xylene	32.14
64	128	dimethylthiophene isomer	0.12
65	129	C_8H_{18} isomer	0.11
66	131	dimethylthiophene isomer	0.26
67	131	styrene	1.80
68	132	C_8H_{18} isomer	0.45
69	132	o-xylene	23.57
70	134	C_8H_{16} isomer	0.15
71	136	anisole	0.09
72	139	C_3-alkyl benzene isomer	0.08
73	139	C_9H_{18} isomer	0.06
74	139	C_3-alkyl benzene isomer	T
75	140	C_9H_{20} isomer	0.11
76	143	C_9H_{20} isomer	T
77	144	$C_{10}H_{22}$ isomer	T
78	146	benzaldehyde	2.65
79	146	C_9H_{18} isomer	0.40
80	147	C_3-alkyl benzene isomer	0.70
81	148	C_9H_{18} isomer	0.78
82	148	C_9H_{20} isomer	
83	149	C_9H_{18} isomer	T
84	150	trimethylthiophene isomer	4.05
85	151	C_9H_{20} isomer	0.30
86	152	phenylpropene	T
87	153	C_3-alkyl benzene isomer	21.00
89	157	C_3-alkyl thiophene isomer	0.25
90	157	methyl cresyl ether	0.13
91	158	$C_{10}H_{20}$ isomer	T
92	159	C_4-alkyl benzene isomer	8.00
93	159	C_3-alkyl benzene isomer	6.00
94	162	indan	16.50
95	163	C_4-alkyl benzene isomer	16.70
96	164	C_4-alkyl benzene isomer	0.12
97	165	C_4-alkyl benzene isomer	T
98	165	indene	0.10
99	166	$C_{10}H_{22}$ isomer	0.11
100	167	C_4-alkyl benzene isomer	0.11
101	169	C_4-alkyl benzene isomer	0.12
102	169	methylindan isomer	0.09

(continued)

Table C13 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
103	170	$C_{10}H_{22}$ isomer	T
104	171	methylindan isomer	0.06
105	171	C_4-alkyl benzene isomer	0.06
106	172	methylbenzofuran isomer	0.05
107	173	C_5-alkyl benzene isomer	0.05
108	174	methylbenzofuran isomer	0.28
109	175	C_5-alkyl benzene isomer	3.10
110	175	$C_{11}H_{22}$ isomer	T
111	177	$C_{10}H_{20}$ isomer	0.04
112	177	C_4-alkyl benzene isomer	0.02
113	178	C_4-alkyl benzene isomer	0.10
114	178	$C_{11}H_{22}$ isomer	T
115	179	C_4H_7-benzene isomer	T
116	180	C_5-alkyl benzene isomer	T
117	182	methylindan isomer	1.92
118	182	C_5-alkyl benzene isomer	T
120	183	$C_{11}H_{22}$ isomer	T
121	183	methylindene isomer	1.35
122	183	C_4H -benzene isomer	0.50
123	184	C_4-alkyl benzene isomer	2.15
124	185	methylindene isomer	T
125	186	C_5-alkyl benzene isomer	T
126	186	C_5-alkyl benzene isomer	T
127	190	naphthalene	54.00
128	190	$C_{11}H_{24}$ isomer	0.65
129	190	C_6-alkyl benzene isomer	1.21
130	190	dimethylindene isomer	3.20
131	191	dimethylindene isomer	T
132	192	C_4-alkyl benzene isomer	T
133	193	C_6-alkyl benzene isomer	0.21
134	194	C_5H_9-benzene isomer	1.21
135	195	C_5-alkyl benzene isomer	0.32
136	198	C_6-alkyl benzene isomer	0.08
137	199	C_6H_{11}-benzene isomer	T
138	200	C_6H_{11}-benzene isomer	0.03
139	201	C_6H_{11}-benzene isomer	T
140	201	C_6-alkyl benzene isomer	0.08
141	203	naphthol (tent.)	0.11
142	204	C_5H_9-benzene isomer	T
143	205	C_6H_{11}-benzene isomer	T
144	206	C_5-alkyl benzene isomer	0.18
145	208	β-methylnaphthalene	2.20
146	208	$C_{13}H_{28}$ isomer	T
147	209	C_7-alkyl benzene isomer	T
148	209	C_6H_{11}-benzene isomer	T
149	211	α-methylnaphthalene	1.35
150	211	C_6H_{11}-benzene isomer	T
151	213	C_6H_{11}-benzene isomer	T
152	214	C_7-alkyl benzene isomer	T
153	215	C_7H_{13}-benzene isomer	T
154	218	C_7-alkyl benzene isomer	T
155	218	C_7H_{13}-benzene isomer	T
156	219	$C_{14}H_{26}$ isomer	T
157	220	biphenyl	45
158	221	C_7H_{13}-benzene isomer	T
159	222	$C_{13}H_{28}$ isomer	0.22
160	223	diphenylmethane	T
161	223	$C_{14}H_{20}$ isomer	0.95
162	224	benzylthiophene (tent.)	T
163	225	C_2-alkyl naphthalene isomer	T
164	228	C_2-alkyl naphthalene isomer	0.05
165	231	C_2-alkyl naphthalene isomer	T
166	233	C_8H_{15}-benzene isomer	0.03
167	240	C_8H_{15}-benzene isomer	0.11
168		dibenzofuran (tent.)	0.13
169		C_3-alkyl naphthalene isomer	T
170		C_3-alkyl naphthalene isomer	T
171		C_3-alkyl naphthalene isomer	T
172		C_3-alkyl naphthalene isomer	0.04
173		C_3-alkyl naphthalene isomer	0.04
174		fluorene	0.07
175		C_3-alkyl naphthalene isomer	0.06

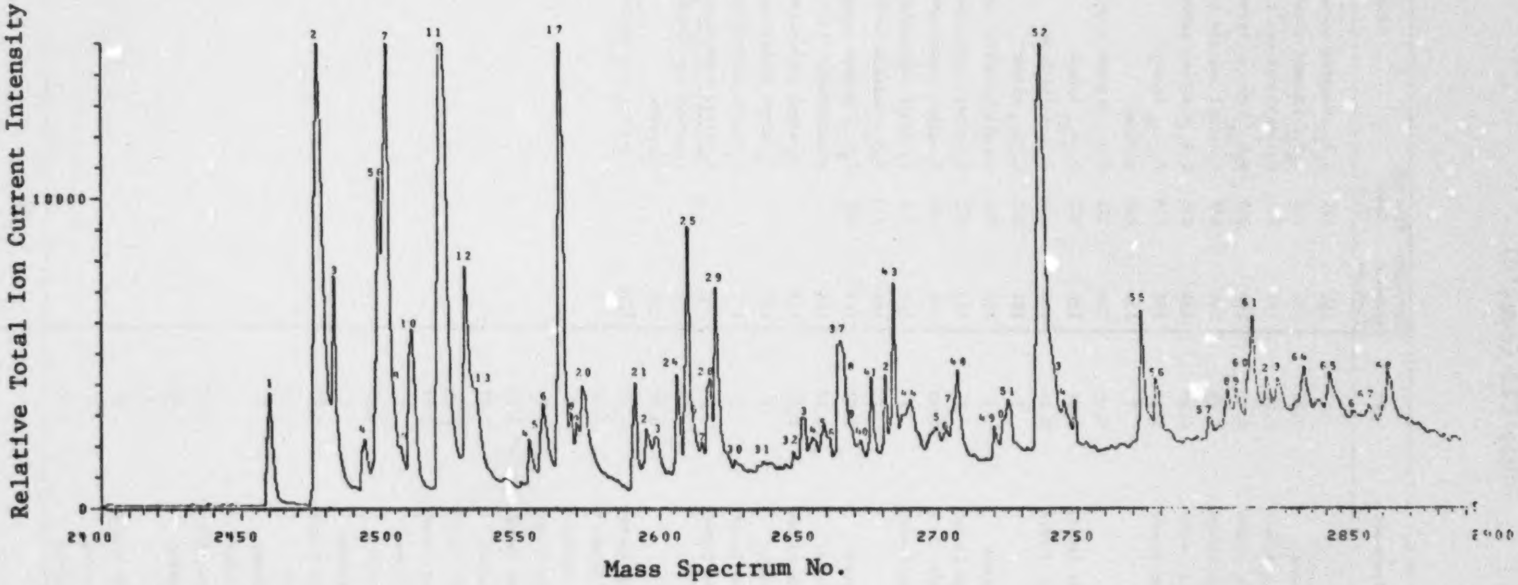


Figure C6. Profile of volatile organics in process water (-3L) from _in situ_ coal gasification (LLL, ERDA).

Table C14. VOLATILE ORGANICS IN PROCESS WATER (-3L) FROM IN SITU COAL GASIFICATION (LLL, ERDA)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
1	49	CO_2	-
1A	52	*n*-propane	NQ
1B	53	1-butene	NQ
1C	54	*n*-butane	T
1D	54	2-butene	NQ
1E	57	acetaldehyde	59.45±8.6
2	58	acetone	2226±334
2A	58	acetonitrile	1246±150
2B	60	C_2H_6S isomer	T
3B	62	cyclopentadiene or C_5H_6 isomer + carbon disulfide (tent.)	T NQ
3C	65	C_4H_8O isomer	9±5.3
3D	66	2-methylpentane	11.02±3.3
4	67	propionitrile	175.3±22.3
4A	68	3-methylpentane	35±13
5	69	methyl ethyl ketone	44.4±5.0
6	70	hexafluorobenzene (e#)	
7	71	*n*-hexane	211±16.7
9	74	isobutyronitrile	34±11
10	76	perfluorotoluene (e#)	
10A	77	methylcyclopentane	17.3±6.0
10C	80	methacrylonitrile (tent.)	T
10D	81	methyl isopropyl ketone	89±33
11	81	benzene	4318±1154
11A	82	thiophene	241±29
12	85	2-pentanone	846±3.6
13	87	3-pentanone	297±3.6
13A	92	α-methylbutyronitrile	T
13B	95	N-methylpyrrole	12±4
14	97	4-methyl-2-pentanone	48±8.3
14A	98	pyrrole	111±11
15	99	2-methyl-3-pentanone	68.5±8.3
16	100	3-methyl-2-pentanone	79±25
16A	102	*n*-pentylnitrile	38±12.6
17	103	toluene	1081±298
17A	104	2-methylthiophene	56±7
18	105	3-methylthiophene	50±11
19	106	3-hexanone	61±6
20	107	2-hexanone	7.3±6
20A	109	cyclopentanone	T
20B	110	C_9H_{20} isomer	T
20C	113	C_8H_{14} isomer	T
21A	117	$C_7H_{14}O$ isomer + 3-methylpyrrole	12.7±6
22	118	2-methylcyclopentanone	55.8±36
22A	119	2-methylpyrrole	26.7±7.3
23	120	3-methylcyclopentanone + $C_7H_{14}O$ isomer	50±21
23A	123	dimethylpyrrole isomer	17±5.7
24	124	ethylbenzene	41±14.0
24A	124	*n*-hexylnitrile + ethylthiophene isomer	41±13.7
25	125	*p* or *m*-xylene	121±14
26	126	dimethylthiophene isomer	14±4
26A	127	2-methylpyridine	33±3
27	128	3-heptanone	62±10.7
27A	128	dimethylthiophene isomer	13.4±3.3
28	129	2-heptanone	40±7
28A	129	styrene	55±27
28B	130	$C_7H_{12}O$ isomer	14±3.3
29	130	*o*-xylene	82±22
29A	132	dimethylthiophene isomer	5.3±2.0
30	135	anisole	5.7±1.7
30A	135	methylpyridine isomer	16.4±2.3
30B	136	dimethylpyrrole isomer	9.3±4.7
30C	137	$C_{10}H_{22}$ isomer	14.4±3.3
30D	138	isopropylbenzene	T
31	139	dimethylpyridine isomer	T
31A	141	C_8H_{16} isomer (tent.)	T
31B	142	methylpyridine isomer	T
32	145	*n*-propylbenzene	6.7±1.7
32A	145	benzaldehyde	19.7±5
32B	146	C_3-alkyl thiophene isomer	5±2
33	146	*m* or *p*-ethyltoluene	54.8±6
34	148	1,3,5-trimethylbenzene	27.4±7
34A	148	$C_{10}H_{22}$ isomer	5±1.7
34B	149	cyanobenzene	23.7±5
35	149	*o*-ethyltoluene	34.0±6.7
36	150	2-octanone	29.7±5
36A	152	$C_{10}H_{22}$ isomer	5±4
37	153	benzofuran	6.3±1.7
37A	153	1,2,4-trimethylbenzene	35.4±5
38	154	phenol	NQ
40	157	$C_8H_{10}O$ isomer	66±6
41	159	1,2,3-trimethylbenzene	41.7±14
42	161	indan	71.8±29
43	162	indene	140±17
43A	164	cresol isomer	NQ
43B	165	C_4-alkyl benzene isomer	25±2.3
44	166	acetophenone	21±5
44A	167	cresol isomer	NQ
44B	169	C_4-alkyl benzene isomer	3.7±3

(continued)

Table C14 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
45	170	C_4-alkyl benzene isomer	T
45A	170	$C_{10}H_{12}$ isomer	T
46	172	C_9H_8O isomer	25.7±3
47	173	C_2-alkyl phenol isomer	NQ
48	174	methylbenzofuran isomer	29.3±5.3
48A	177	cresol + C_4-alkyl benzene isomers	NQ
48B	179	dimethyl phenol isomer	NQ
49	181	$C_{10}H_{12}$ + C_2-alkyl phenol isomers	NQ
50	182	methylindene isomer	37.7±8.7
51	183	C_4-alkyl benzene isomer	T
51B	184	C_2-alkyl phenol isomer	NQ
51C	186	C_2-alkyl phenol isomer	NQ
51D	187	C_3-alkyl phenol isomer	NQ
51E	188	2-decanone	7.3±2
52	189	naphthalene	1707±79
52A	190	benzothiophene	39.4±8.6
53	192	dimethylbenzofuran isomer	20.7±3.3
54	193	dimethylbenzofuran isomer	31.4±5
54A	200	C_3-alkyl indan isomer	12.6±6.7
54B	201	*n*-hexylbenzene	T
54C	202	methyldihydronaphthalene isomer	T
54D	204	methylbenzimidazole isomer	T
54E	205	C_2-alkyl indan isomer	7±3.3
54F	206	C_3-alkyl indan isomer	5±3
55	207	β-methylnaphthalene	66±12.4
55A	209	C_3-alkyl indan isomer	12.7±5.7
56	210	α-methylnaphthalene	77.8±15.4
56A	214	$C_{12}H_{16}$ isomer	T
56B	215	$C_{13}H_{18}$ isomer	T
56C	216	$C_{12}H_{16}$ isomer	T
56D	217	C_7-alkyl benzene isomer	T
56E	217	$C_{12}H_{16}$ isomer	T
57	219	biphenyl	30.7±10.3
57A	220	$C_{14}H_{28}$ isomer	3.3±1.7
57B	221	*n*-tetradecane	11.3±2.3
58	222	ethylnaphthalene isomer	19.7±7
59	224	dimethylnaphthalene isomer	55±9
59A	225	$C_{13}H_{18}$ isomer	T
60	226	dimethylnaphthalene isomer	12.7±1.7
61	227	dimethylnaphthalene isomer	49±63
62	230	dimethylnaphthalene isomer	74±16.7
63	232	biphenylene	21±1.7
63A	235	$C_{15}H_{30}$ isomer	T
64	237	acenaphthene + *n*-pentadecane	31.4±5.3
64A	239	C_3-alkyl naphthalene isomer	T
64B	240	C_3-alkyl naphthalene isomer	T
65	240	dibenzofuran	T
65A	240	$C_{14}H_{20}$ isomer	1.4±0.7
65B	240	C_3-alkyl naphthalene isomer	6±3
66	240	trimethylnaphthalene isomer	10.7±1.4
67	240	C_3-alkyl naphthalene isomer	11.7±3.7
67A	240	$C_{14}H_{20}$ isomer	T
67B	240	$C_{16}H_{32}$ isomer	T
68	240	fluorene	18±16.7
68A	240	*n*-hexadecane	11.4±2
68B	240	trimethylnaphthalene isomer	48±5.7
68C	240	propylnaphthalene isomer	T
68D	240	C_4-alkyl naphthalene isomer (tent.)	NQ
68E	240	$C_{13}H_{10}O$ or $C_{14}H_{14}$ isomer	NQ
68F	240	C_4-alkyl naphthalene isomer	NQ
68G	240	$C_{15}H_{22}$ isomer	NQ

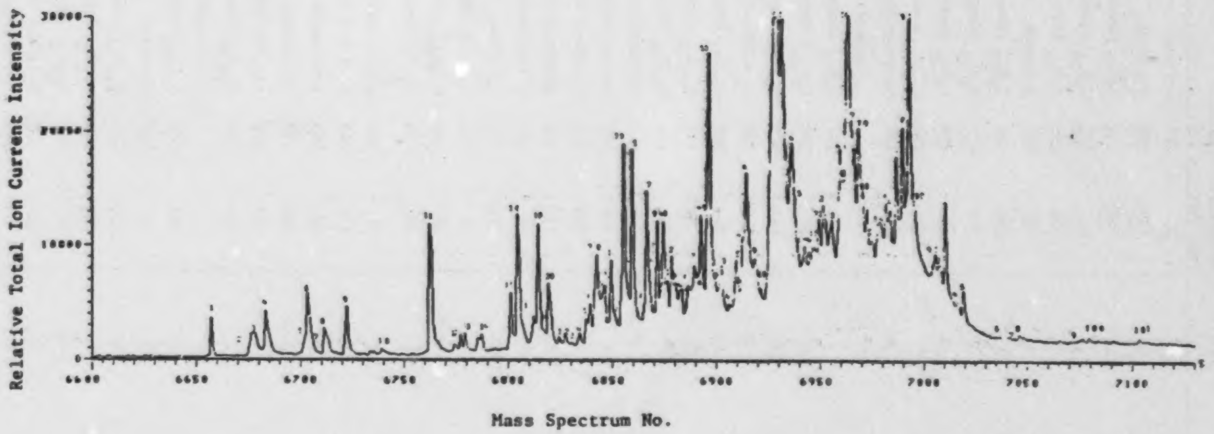


Figure C7. Profile of volatile organics in product tar (-4T) from in situ coal gasification (LLL, ERDA).

Table C15. VOLATILE ORGANICS IN PRODUCT TAR (-4T) FROM IN SITU COAL GASIFICATION (LLL, ERDA)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppm
1	50	CO_2	-
1A	54	1-butene	NQ
1B	55	n-butane	NQ
2	59	acetaldehyde	T
3	61	acetone	31
3A	62	propenal + propanal	NQ
4B	68	ter-butanol (tent.)	T
4C	71	2-methylpentane	5
4D	72	3-methylpentane	3
5	73	hexafluorobenzene (e[illegible])	
6	74	n-hexane	250
7A	77	butanal	T
8	78	perfluorotoluene (e[illegible])	
8A	79	methylcyclopentane	43
9	82	benzene	272
9A	83	thiophene	5
9C	89	C_7H_{16} isomer	T
9D	90	n-pentanal	T
9E	91	C_7H_{14} isomer	T
10	91	n-heptane	1.2
10A	96	C_7H_{14} isomer	T
10B	99	4-methyl-2-pentanone	T
10C	100	$C_6H_{12}O$ isomer	T
10D	101	C_7H_{12} isomer	T
11	103	toluene	1018
11A	104	C_8H_{18} isomer	T
11B	105	2-methylthiophene	12.4
11C	108	3-hexanone	T
12	109	C_8H_{16} isomer	T
12A	110	2-hexanone	12.4
12B	111	C_8H_{16} isomer	30
13	112	n-octane	22.4
13A	113	C_8H_{16} isomer	T
13C	114	C_8H_{14} isomer	T
14A	118	C_9H_{20} isomer	T
14B	119	C_9H_{18} isomer	T
14D	120	C_9H_{18} isomer	T
14E	121	C_8H_{14} isomer	T
14F	122	C_9H_{18} isomer	T
15	123	ethylbenzene	100
15A	124	ethylthiophene isomer	35
15B	124	C_9H_{16} isomer	T
16	125	m or p-xylene	628
16A	126	dimethylthiophene isomer	41.2
16B	127	C_9H_{20} isomer	30
16C	128	dimethylthiophene isomer	44
17	129	styrene	107
18	130	o-xylene	429
18A	130	C_9H_{18} isomer	20
19	131	C_9H_{18} isomer	T
19A	132	C_9H_{16} isomer	160
20	132	n-nonane	200
20A	133	C_9H_{18} isomer	43
20B	134	C_9H_{16} isomer	T
21	135	C_9H_{18} isomer	T
21A	135	$C_{10}H_{20}$ isomer	T
22	136	isopropylbenzene + $C_{10}H_{22}$ isomer	67.8
22A	137	C_9H_{16} isomer	T
23	138	$C_8H_{16}O$ isomer	T
23A	139	$C_{10}H_{20}$ isomer	T
23B	139	C_3-alkyl cyclohexane isomer	57.6
24	140	$C_{10}H_{22}$ isomer	T
24A	140	$C_{10}H_{20}$ isomer	35
25	141	$C_{10}H_{22}$ isomer	T
26	142	n-propylbenzene	44
26A	143	benzaldehyde	50
26B	143	C_3-alkyl thiophene isomer	T
27	144	m-ethyltoluene	367
28	144	p-ethyltoluene	175
28A	145	C_3-alkyl thiophene isomer	T
29	145	1,3,5-trimethylbenzene	50
30	146	$C_{11}H_{24}$ isomer	122
30A	146	$C_{10}H_{18}$ isomer	T
31	147	o-ethyltoluene	571
31A	148	C_3-alkyl thiophene isomer	T
32	148	2-octanone	68.4
32A	150	benzofuran + $C_{10}H_{20}$ isomer	250
33	150	1,2,4-trimethylbenzene	928
34	151	$C_{10}H_{20}$ isomer + silane compound (BKG)	280
34A	152	$C_{10}H_{18}$ isomer	T
35	152	n-decane	1200
35A	153	$C_{10}H_{20}$ isomer	T
35B	154	$C_{11}H_{22}$ isomer	T
36	155	$C_{10}H_{20}$ isomer	T
36A	155	C_4-alkyl benzene isomer	181
37	156	1,2,3-trimethylbenzene	833
37A	156	C_4-alkyl benzene isomer	T
38	157	$C_{11}H_{24}$ isomer	T
38A	158	$C_{11}H_{24}$ isomer	T
39	158	indan	533

(continued)

Table C15 (cont'd)

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	ppm
39A	159	$C_{11}H_{22}$ isomer	T
39B	159	C_4-alkyl cyclohexane isomer	T
40	160	indene	833
40A	160	*o*-cymene + $C_{11}H_{22}$ isomer	86.6
41	161	*p*-propyltoluene	167
42	162	*n*-butylbenzene	6.6
43	163	$C_{11}H_{22}$ + C_4-alkyl thiophene isomers	T
43A	163	acetophenone	100
44	164	*o*-propyltoluene	53.4
44A	165	$C_{11}H_{20}$	T
45	165	methylindan + C_4-alkyl benzene + $C_{11}H_{22}$ isomers	280
46	166	dimethylethylbenzene isomer	100
47	168	methylindan isomer + 2-nonanone	300 100
48	169	$C_{10}H_{12}$ isomer	50
48A	169	dimethylethylbenzene isomer	36.6
49	170	$C_{11}H_{22}$ isomer	35.2
49A	170	dimethylstyrene or $C_{10}H_{12}$ isomer	T
49B	171	cresol isomer	NQ
50	171	*n*-undecane	828
50A	172	methylbenzofuran isomer	400
51	173	C_5-alkyl benzene isomer	T
51A	173	$C_{11}H_{22}$ isomer	T
52	174	$C_{12}H_{26}$ + methylbenzofuran isomers	125
53	175	1,2,4,5-tetramethylbenzene	168
53A	175	$C_{10}H_{12}$ isomer	13
53B	176	C_5-alkyl benzene isomer	T
53C	176	$C_{11}H_{14}$ + $C_{12}H_{24}$ isomers	T
54	177	C_5-alkyl benzene isomer	T
54A	177	C_4-alkyl benzene isomer	T
54B	178	$C_{12}H_{24}$ isomer	T
55	178	$C_{10}H_{12}$ isomer	T
56	179	C_5-alkyl benzene + C_5-alkyl cyclohexane isomers	T T
56A	179	$C_{12}H_{24}$ isomer	T
57	180	methylindene isomer	28
57A	180	methylindan isomer	T
58	181	1,2,3,5-tetramethylbenzene + *n*-pentylbenzene	182 125
58A	181	$C_{12}H_{26}$ isomer	42
58B	182	C_5-alkyl benzene isomer	41
58C	182	$C_{12}H_{24}$ isomer	T
59	183	C_5-alkyl benzene isomer	102
59A	184	methylindene isomer	T
60	184	C_5-alkyl benzene isomer	T
60A	185	dimethylindan isomer	T
60B	185	$C_{12}H_{24}$ isomer	T
60C	186	2-decanone	100
61	186	naphthalene	13920
61A	188	dimethylindan + $C_{12}H_{24}$ isomers	107
61B	188	$C_{10}H_{14}$ isomer	T
61C	189	$C_{11}H_{14}$ isomer	T
62	189	*n*-dodecane	1120
63	191	C_6-alkyl benzene isomer	T
63A	191	dimethylbenzofuran isomer	240
64	192	$C_{13}H_{28}$ isomer	162
65	192	C_6-alkyl benzene + $C_{13}H_{26}$ isomers	T
66	193	C_3-alkyl indan isomer	T
66A	194	$C_{13}H_{26}$ isomer	T
67	195	$C_{11}H_{14}$ isomer	T
67A	195	$C_{12}H_{16}$ isomer	T
68	196	$C_{13}H_{28}$ isomer	T
68A	196	$C_{13}H_{26}$ + $C_{12}H_{16}$ isomer	T
69	197	C_6-alkyl cyclohexane + C_6-alkyl benzene isomers	T
69A	197	$C_{13}H_{26}$ + $C_{12}H_{16}$ isomers	T
70	198	C_6-alkyl benzene isomer	17.6
70A	198	*n*-hexylbenzene	56.6
71	199	3-methyl-1,2-dihydronaphthalene	116
71A	199	C_6-alkyl benzene + $C_{13}H_{28}$ isomers	82
72	200	C_3-alkyl indan isomer	T
72A	200	$C_{11}H_{12}$ isomer	22
73	201	$C_{14}H_{30}$ isomer	65
73A	202	2-nonanone	T
73B	203	$C_{11}H_{14}$ isomer	T
74	203	$C_{13}H_{26}$ isomer	37.8
75	204	trimethylindan + $C_{14}H_{28}$ isomer	6.6
76	205	*n*-tridecane + β-methylnaphthalene	675
77	206	$C_{14}H_{28}$ isomer	933
78	207	trimethylindan + $C_{13}H_{26}$ isomer	128
79	208	α-methylnaphthalene	867
80	209	C_3-alkyl indan isomer	T
80A	209	C_4-alkyl indan + C_7-alkyl benzene isomers	T

(continued)

Table C15 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppm	Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
81	210	C_3-alkyl indan isomer	T			
82	211	C_7-alkyl benzene isomer	T			
82A	211	C_4-alkyl indan isomer	T			
82B	212	C_8-alkyl benzene + C_4-alkyl indan isomers	12			
83	212	2,6-dimethyl-1,2,3,4-tetrahydronaphthalene	210			
83A	213	$C_{14}H_{28}$ isomer	T			
84	213	$C_{15}H_{30}$ isomer	28.8			
85	214	*n*-heptylbenzene + $C_{14}H_{30}$ isomer	100			
85A	215	C_4-alkyl indan isomer	85			
86	216	dimethylfluorene isomer	5			
86A	217	$C_{14}H_{28}$ + C_4-alkyl indan isomer	T			
87	218	$C_{15}H_{32}$ isomer	110			
88	219	$C_{14}H_{28}$ isomer	43			
88A	220	methylphenanthrene isomer	54.2			
88B	220	$C_{15}H_{30}$ isomer	T			
89	221	*n*-tetradecane	625			
90	222	$C_{15}H_{30}$ isomer	T			
90A	224	$C_{16}H_{34}$ isomer	T			
90B	226	$C_{15}H_{24}$ isomer	T			
91	227	4,5-dimethylphenanthrene	5			
91A	227	*n*-nonylbenzene	22.8			
92	229	$C_{16}H_{32}$ isomer	10			
93	230	$C_{16}H_{34}$ isomer	126			
94	233	$C_{15}H_{30}$ isomer	T			
95	234	*n*-pentadecane	200			
95A	236	$C_{16}H_{34}$ isomer	T			
95B	237	$C_{16}H_{32}$ isomer	T			

Table C16. VOLATILE ORGANICS IN WATER (-5L) FROM PERMEATION WELL #5 (LLL, ERDA)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
1	50	CO_2	-
1A	55	n-butane	NQ
2	62	acetaldehyde	T
2A	63	n-pentane + furan	1.10±0.3
2B	64	propanal + propenal	1.00±0.3
4A	68	acetone	2.30±0.8
5	71	2-methylpentane	8.68±1.8
6	73	3-methylpentane	3.64±1.9
7	74	hexafluorobenzene (e[illegible])	
8	75	n-hexane	32.42±11.0
10	80	perfluorotoluene (e[illegible])	
10A	81	methylcyclopentane	5.64±0.3
11	85	benzene	3.72±0.9
11B	86	cyclohexane	T
11C	89	$C_5H_{10}O$ isomer	T
11D	90	C_7H_{16} isomer	T
12A	94	C_7H_{16} isomer	T
12B	98	C_7H_{14} isomer	T
12C	99	C_7H_{14} isomer	T
13	105	toluene	11.32±1.3
14	112	$C_6H_{12}O$ isomer	T
14A	114	n-octane	T
14C	122	C_6H_8O isomer	T
14D	124	C_9H_{18} isomer	T
14E	125	C_9H_{20} isomer	T
14F	125	ethylbenzene	T
14G	127	p or m-xylene	T
14H	130	C_9H_{20} isomer	0.78±0.3
15	131	C_9H_{20} isomer	T
15A	131	styrene	0.62±0.1
15B	132	$C_{10}H_{20}$ isomer	T
16	133	o-xylene	0.64±0.1
16A	134	C_9H_{18} isomer	T
16B	135	C_9H_{20} isomer	T
17	136	n-nonane	T
18	140	$C_{10}H_{22}$ isomer	0.30±0.1
19	143	$C_{10}H_{22}$ isomer	0.20±0
19A	145	$C_{10}H_{20}$ isomer	T
20	147	benzaldehyde	1.46±0.2
20A	148	$C_{10}H_{22}$ isomer	T
20B	149	p-ethyltoluene	1.22±0.3
21	150	$C_{11}H_{24}$ isomer	1.92_0.5
21A	151	cyanobenzene	0.56±0.2
22	152	$C_{11}H_{24}$ isomer	T
22A	155	$C_8H_{16}O$ isomer	T
24	156	n-decane	0.44±0.2
24A	157	phenol	NQ
25	159	1,2,3-trimethylbenzene	0.56±0.2
25A	160	$C_{11}H_{24}$ isomer	T
25B	162	$C_{12}H_{26}$ isomer	T
26	165	$C_{12}H_{26}$ + C_4-alkyl benzene isomers	0.30±0.1
27	166	C_4-alkyl benzene isomer	T
27A	166	C_4-alkyl benzene isomer	T
27B	167	$C_{11}H_{24}$ isomer	
28	167	acetophenone	1.02±0.3
29	171	C_4-alkyl benzene isomer	T
29A	172	$C_{10}H_{12}$ isomer	T
30	173	$C_{11}H_{22}$ isomer	T
31	175	n-undecane	T
31A	176	C_4-alkyl benzene isomer	T
31B	176	$C_{12}H_{26}$ isomer	T
31C	177	$C_{12}H_{24}$ isomer	T
32	178	tetramethylbenzene isomer	T
32A	179	$C_{12}H_{26}$ isomer	T
32B	181	C_5-alkyl benzene isomer	T
32C	183	$C_{10}H_{12}$ isomer	T
32D	184	tetramethylbenzene isomer	T
33A	188	2-decanone	0.40±0.2
34	189	naphthalene	4.70±1.0
36	191	C_5-alkyl benzene isomer	0.36±0.2
36A	191	n-dodecane	T
36B	192	dimethylindan isomer	T
36C	194	$C_{12}H_{24}$ isomer	T
36D	206	$C_{13}H_{26}$ isomer	T
36E	207	β-methylnaphthalene	0.36±0.1
37	208	n-tridecane	T
37A	210	$C_{13}H_{26}$ isomer	T
37B	211	α-methylnaphthalene	T
38	223	n-tetradecane	0.22±0.1
38A	224	$C_{14}H_{28}$ isomer	T

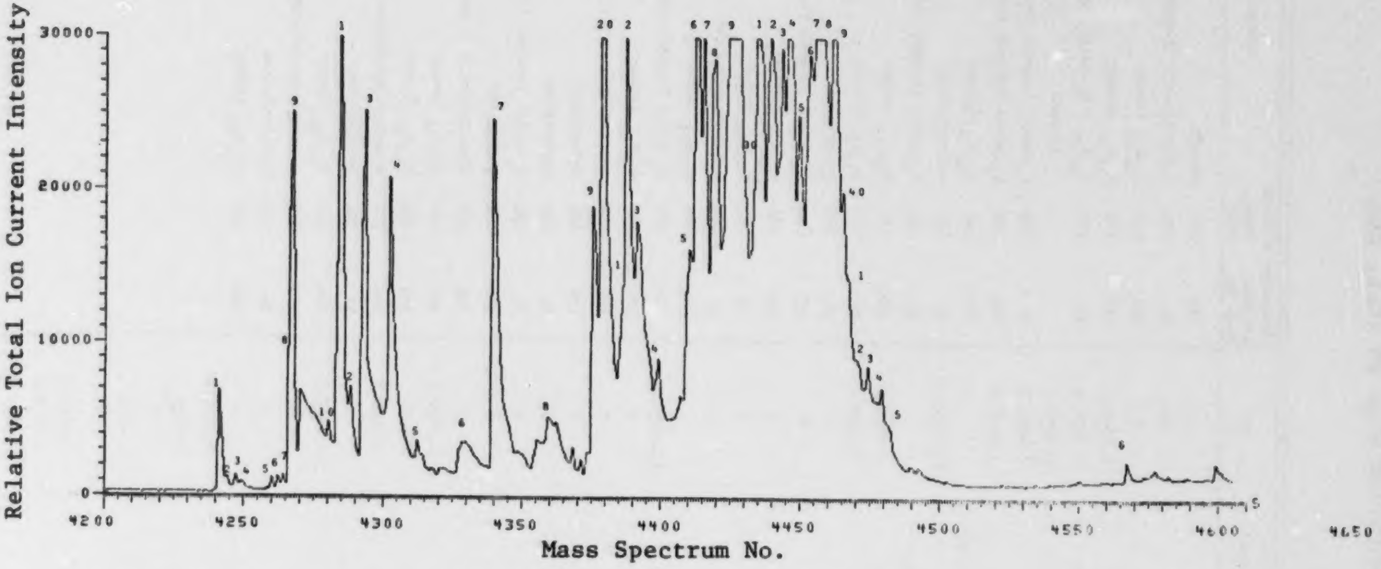


Figure C8. Profile of volatile organics in liquid process composite (-6L) from in situ coal gasification (LLL, ERDA).

Table C17. VOLATILE ORGANICS IN LIQUID PROCESS COMPOSITE (-6L) FROM IN SITU COAL GASIFICATION (LLL, ERDA)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
1A	41	CO_2	-
2	42	carbonyl sulfide	NQ
3	45	sulfur dioxide	NQ
4	45	C_4H_8 isomer	NQ
5A	51	C_5H_{10} isomer	T
6	51	_n_-pentane	8.68 ± 1.7
6A	52	furan	5.68 ± 2.3
7	52	acetaldehyde	20.37 ± 5.0
8	53	C_5H_{10} isomer	T
9A	55	propanal	300 ± 42
9B	57	acetone + acetonitrile	187 ± 9.7
10	61	C_6H_{14} isomer	70 ± 17
11	63	perfluorobenzene (e#)	
11A	63	_n_-hexane	180 ± 32
13	67	perfluorotoluene (e#) + methylcyclopentane	11.69 ± 3.3
13A	68	2-butanone	6.01 ± 2.4
14	72	benzene	707 ± 18
14A	73	thiophene	26 ± 3.7
15A	78	C_7H_{16} isomer	17.7 ± 5.3
15B	80	_n_-heptane	3.67 ± 1.4
15C	81	methyl isopropyl ketone	40 ± 12.7
16	85	2-pentanone	132 ± 43
16A	86	3-pentanone (tent.)	9.35 ± 3.3
17	90	toluene	967 ± 100
17A	93	methylthiophene + $C_6H_{12}O$ isomers	29 ± 6.3
17B	93	C_8H_{16} isomer	T
17C	94	_n_-octane	14 ± 3.3
17D	95	_n_-pentylnitrile	32 ± 5.7
17E	95	3-hexanone	13.7 ± 2.7
18	97	2-hexanone	604 ± 125
18A	106	3-methyl acetylacetone (tent.)	6 ± 6
18B	107	$C_7H_{14}O$ ketone isomer	T
19	108	ethylbenzene	585 ± 60
19A	109	ethylthiophene + $C_7H_{14}O$ ketone isomers	24 ± 3.3
20	109	xylene + dimethylthiophene isomers	981 ± 176
21	113	dimethylthiophene isomer	14.7 ± 3
22	114	dimethylthiophene + xylene isomers	848 ± 180
22A	115	C_2-alkyl benzene isomer	8.35 ± 2
22B	116	$C_7H_{14}O$ ketone isomer	T
23	116	C_9H_{18} isomer	191 ± 30
23A	117	2-heptanone	
24	119	C_3-alkyl benzene isomer	72 ± 20
24A	123	C_9H_{20} isomer	T
25	125	C_3-alkyl benzene isomer	131 ± 28
26	126	3-octanone	10 ± 1.7
26A	126	C_3-alkyl benzene isomer	65 ± 13
27	128	C_3-alkyl thiophene isomer	21 ± 7.3
28	129	C_3-alkyl benzene isomer	224 ± 34
28A	130	C_3-alkyl thiophene isomer	25 ± 3.3
29	132	$C_{10}H_{20}$ isomer	137 ± 26
29A	132	C_3-alkyl benzene isomer	255 ± 44
29B	133	benzofuran	225 ± 24
30	133	_n_-decane	8 ± 1.7
30A	134	$C_{10}H_{20}$ isomer	83 ± 10
30B	134	$C_8H_{16}O$ ketone isomer	37 ± 15
30C	135	C_3-alkyl thiophene isomer	14 ± 3
31	137	$C_{10}H_{20}$ isomer	T
31A	137	C_4-alkyl benzene isomer	97 ± 3
31B	138	C_3-alkyl benzene isomer	93 ± 5
32	140	indan	483 ± 127
32A	142	indene	54 ± 24
33	143	$C_{10}H_{20}$ + C_4-alkyl benzene isomers	57 ± 21
34	143	C_4-alkyl benzene isomer	47 ± 21
34A	144	C_4-alkyl thiophene isomer	24 ± 3.3
34B	144	$C_{11}H_{24}$ isomer	29 ± 17
35	145	C_4-alkyl benzene isomer	33 ± 3.3
35A	146	C_4-alkyl thiophene + $C_{11}H_{24}$ isomers	18.7 ± 33
36	147	C_4-alkyl benzene isomer	10.7 ± 5.3
37	148	C_4-alkyl benzene isomer	18.4 ± 5.2
37A	148	$C_{10}H_{12}$ isomer	T
38	149	$C_{11}H_{22}$ isomer	T
39	151	C_5-alkyl benzene + methyl-benzofuran isomer	25 ± 6.7
39A	152	_n_-undecane	151 ± 16
40	153	C_5-alkyl benzene isomer	T
40A	153	$C_{11}H_{22}$ isomer	T
41	153	C_5-alkyl benzene isomer	29 ± 3
41A	154	$C_{12}H_{26}$ isomer	T
42	155	$C_{12}H_{26}$ isomer	19 ± 5
42A	156	$C_{12}H_{22}$ isomer	T
42B	157	$C_{11}H_{22}$ isomer	T
43	157	$C_{12}H_{24}$ isomer	T
44	160	C_5-alkyl benzene isomer	23 ± 5.7
44A	160	C_6-alkyl phenol isomer	NQ

(continued)

Table C17 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb	Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
45	161	C_5-alkyl benzene isomer	4 ± 1.7			
45A	164	$C_{12}H_{24}$ isomer	T			
45B	165	naphthalene	1653 ± 367			
45C	165	*n*-dodecane	4 ± 1.7			
46A	209	$C_{15}H_{24}O$ isomer	6.3 ± 3.3			

Table C18. VOLATILE ORGANICS IN LIQUID PROCESS COMPOSITE (-7L) FROM *IN SITU* COAL GASIFICATION (LLL, ERDA)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
1	40	CO_2	-
1A	40	carbonyl sulfide	NQ
1B	42	C_4H_{10} isomer	NQ
1C	42	C_4H_8 isomer	T
1D	43	*n*-butane	T
1E	46	isopentane	T
2A	47	C_5H_{12} isomer + furan	T
3	49	acetaldehyde	26.7±8.7
3A	49	C_5H_{10} isomer	T
4	50	acetone + acetonitrile (tent.)	539±151
5	55	C_6H_{14} isomer	19.7±3.3
6	57	perfluorobenzene (e[illegible])	
6A	57	*n*-hexane	417±112
7A	60	*n*-butanal	T
8	61	perfluorotoluene (e[illegible])	
8A	62	methylcyclopentane	8.3±3
8B	62	methyl ethyl ketone	498±224
9	65	benzene	1205±53
9A	67	thiophene	75±22
10	73	methyl isopropyl ketone	196+24
10A	74	C_7H_{16} isomer	T
10B	76	*n*-butyronitrile	93±23
11	77	2-pentanone	542±97
11A	85	C_7H_{12} isomer	11.7±1.7
12	85	4-methyl-2-pentanone	74±26
13	86	toluene	1554±286
14	89	methylthiophene isomer	68±25
14A	91	methylthiophene isomer	67±20
14B	91	3-methyl-2-pentanone	21±5
15	93	C_8H_{16} isomer	T
15A	94	*n*-pentylnitrile	331±42
15B	95	*n*-octane	170±33
15C	96	C_8H_{16} isomer	44±21
15D	98	$C_6H_{12}O$ ketone isomer	107±25
15E	102	C_8H_{16} isomer	T
15F	103	C_9H_{18} isomer	T
15G	105	C_9H_{18} isomer	22±5
16	105	$C_7H_{14}O$ ketone isomer	9.35±3.6
17	106	ethylbenzene + ethylthiophene isomer	1423±259
18	108	dimethylthiophene + xylene isomers	2000±452
19	109	dimethylthiophene isomer	87±23
20	111	dimethylthiophene isomer	60±33
21	112	*o*-xylene	1215±330
21A	113	C_9H_{18} isomer	38±12
22A	116	$C_7H_{14}O$ isomer	NQ
23	117	C_9H_{18} isomer	114±39
24	119	isopropylbenzene	20±5.7
25	122	C_9H_{18} isomer	164±39
25A	122	$C_{10}H_{22}$ isomer	T
26	123	$C_{10}H_{22}$ isomer	T
26A	124	C_9H_{16} isomer	72±29
27	125	C_3-alkyl benzene isomer	184±36
28	126	C_3-alkyl thiophene + C_3-alkyl benzene isomers	1202±296
29	128	C_3-alkyl benzene + C_3-alkyl thiophene + $C_{10}H_{22}$ isomers	668±172
30	130	C_3-alkyl benzene isomer	835±330
30A	130	C_3-alkyl thiophene isomer	T
31	133	$C_{10}H_{20}$ + C_3-alkyl benzene isomers	892±267
31A	134	$C_{10}H_{20}$ + $C_{10}H_{18}$ isomers + benzofuran	79±33
32	135	*n*-decane	1572±501
32A	135	$C_{10}H_{20}$ isomer	203±110
32B	136	C_3-alkyl thiophene isomer	T
33	137	$C_{11}H_{22}$ + $C_{10}H_{20}$ isomers	154±18
34	138	C_4-alkyl benzene isomer	1068±272
34A	138	C_3-alkyl benzene isomer	1002±167
34B	139	C_4-alkyl benzene isomer	T
34C	140	$C_{11}H_{24}$ isomer	T
35	141	indan	2766±379
35A	141	C_4-alkyl benzene isomer	952±204
35B	142	$C_{10}H_{20}$ isomer	100±33
35C	142	indene	668±167
36	143	C_4-alkyl thiophene + C_4-alkyl benzene isomers	192±37
37	144	C_4-alkyl benzene isomer	501±58
37A	145	C_4-alkyl thiophene isomer	T
38	146	C_4-alkyl benzene isomer	167±3
38A	146	$C_{11}H_{24}$ isomer	205±45
38B	147	C_4-alkyl thiophene isomer	238±67
39	148	C_4-alkyl benzene isomer	718±167
40	149	$C_{10}H_{12}$ isomer	785±139
41	150	$C_{11}H_{22}$ isomer	2171±83
42	153	methylbenzofuran isomer	2371±167
42A	153	C_5-alkyl benzene isomer	671±185
42B	154	*n*-undecane	1277±334
42C	154	methylbenzofuran + C_4-alkyl benzene isomer	2082±568
42D	155	C_4-alkyl benzene isomer	701±150

(continued)

Table C18 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb	Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
43	155	$C_{11}H_{22}$ + C_5-alkyl benzene isomers	100±50			
44	156	C_4-alkyl benzene isomer	501±200			
45	156	$C_{12}H_{26}$ isomer	34±13			
46	157	C_5-alkyl benzene isomer	T			
47	158	$C_{10}H_{12}$ + $C_{11}H_{14}$ isomers	68±17			
47A	159	C_5-alkyl benzene isomer	716±200			
48	160	$C_{10}H_{12}$ isomer	187±33			
48A	161	C_5-alkyl benzene + C_4-alkyl benzene isomers	521±132			
48B	162	methylindene isomer	317±134			
49	163	C_5-alkyl benzene isomer	367±127			
50	165	naphthalene	3849±1002			
51	167	$C_{12}H_{24}$ isomer	217±67			
51A	167	$C_{11}H_{14}$ isomer	92±13			
52	168	*n*-dodecane	1915±271			
53	169	$C_{11}H_{14}$ isomer	209±10			
54	172	$C_{13}H_{28}$ isomer	T			
55	177	$C_{11}H_{12}$ isomer	67±17			
56	181	$C_{11}H_{14}$ isomer	79±23			
57	182	$C_{12}H_{16}$ + $C_{13}H_{26}$ isomers	480±200			
57A	182	β-methylnaphthalene	2826±67			
58	183	*n*-tridecane	362±117			
58A	185	α-methylnaphthalene	2505±668			
58B	186	$C_{12}H_{16}$ isomer	68±33			
58C	201	benzothiophene (tent.)	T			
59	205	dimethylbenzofuran isomer	2532±485			
59A	208	dimethylbenzofuran isomer	2229±501			
59C	217	$C_{13}H_{18}$ isomer	T			
61A	221	*n*-$C_{17}H_{36}$ isomer	39±17			

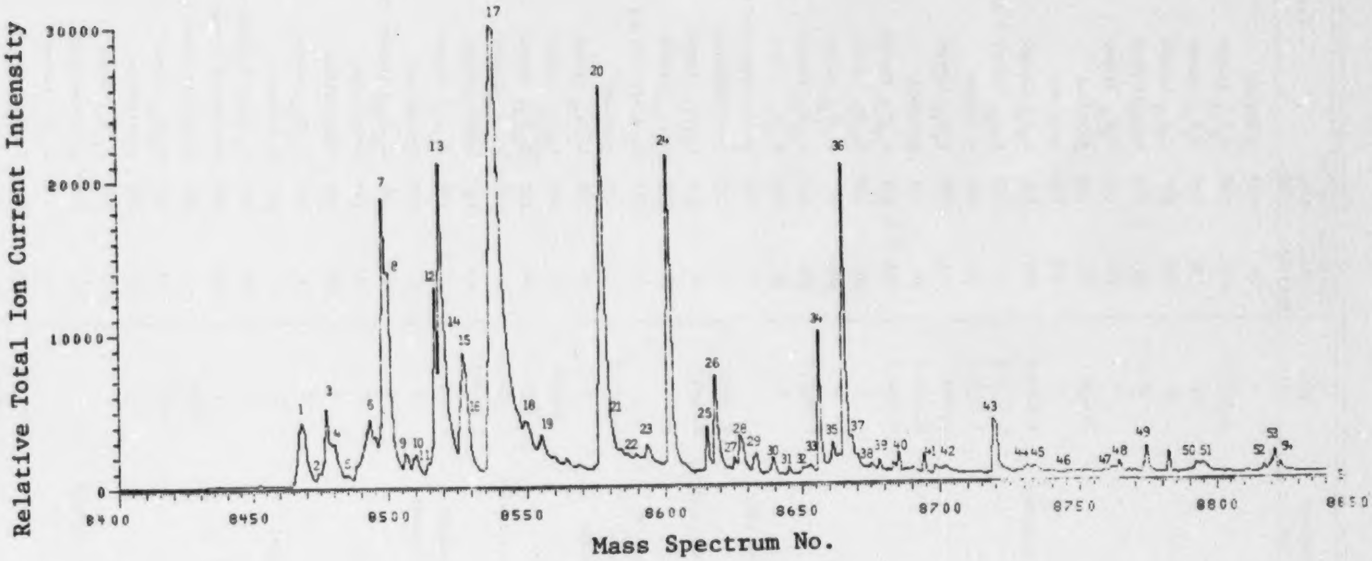


Figure C9. Profile of volatile organics in water sample (-8L) from environmental well #4 (LLL, ERDA).

Table C19. VOLATILE ORGANICS IN WATER SAMPLE (~8L) FROM ENVIRONMENTAL WELL #4 (LLL, ERDA)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
1	54	CO_2	-
2	58	isobutane	3.27±0.5
2A	59	1-butene	NQ
3	59	*n*-butane	NQ
4	60	2-butene	T
4A	63	C_5H_8 isomer	T
5	63	C_5H_{10} isomer	0.17±0
5A	65	isopentane	T
5C	66	C_5H_{10} isomer + propanal	6.50±3.1
5D	67	acetone	0.77±0.2
6	67	*n*-pentane	1.35±0.6
6A	68	C_5H_{10} isomer	0.15±0
9	74	cyclopentane	0.44±0.2
10	76	C_6H_{12} isomer	0.65±0.3
10A	76	C_6H_{14} isomer	T
11	78	3-methylpentane	T
11A	78	*n*-butanal	0.30±0.2
11B	79	C_6H_{12} isomer	T
12	79	hexafluorobenzene (eI)	
13	80	*n*-hexane	4.75±1.1
14A	82	C_6H_{10} isomer + diisopropyl ether (tent.)	0.11±0
15	84	perfluorotoluene (eI)	
16	85	methylcyclopentane	0.42±0.2
16A	87	methyl ethyl ketone	T
17	90	benzene	180±54
17A	91	thiophene	0.72±0.2
18A	96	C_7H_{14} isomer	T
19	98	C_7H_{16} isomer	0.97±0.2
19A	99	C_7H_{14} + C_7H_{12} isomers	0.63±0.1
19B	100	methylhexadiene isomer	T
19C	101	C_7H_{16} isomer	T
19D	102	ethylcyclopentane	T
19E	103	C_7H_{14} isomer	T
19F	105	C_7H_{12} isomer	T
19G	106	$C_5H_{10}O$ isomer (tent.)	T
19H	108	C_7H_{12} isomer	T
19I	108	C_8H_{14} isomer	T
20	109	toluene	80±0
20A	110	C_7H_{14} isomer	0.11±0
21	111	C_8H_{16} isomer	T
21A	112	C_8H_{18} isomer	T
21B	113	hexadiene isomer (tent.)	T
22	115	*n*-hexanal	T
22A	115	C_8H_{16} isomer	1.80±0.3
22B	117	C_8H_{14} isomer	1.00±0.2
23	117	*n*-octane	0.11±0
23A	118	C_8H_{16} isomer	1.31±0.4
23C	119	C_8H_{14} isomer	T
24A	127	C_9H_{18} isomer	T
25	128	ethylbenzene	0.40±0.1
25A	129	C_9H_{16} isomer	T
26	130	*p*-xylene	1.25±0.5
26A	131	*m*-xylene	0.12±0
26B	131	C_9H_{18} isomer	T
27	133	C_9H_{20} isomer + styrene	T
28	134	*o*-xylene	0.07±0
28A	135	C_9H_{18} isomer	T
29	137	*n*-nonane	4.11±0.7
29A	139	$C_{10}H_{20}$ isomer	T
30	140	$C_{10}H_{22}$ isomer	0.75±0.1
30A	141	$C_{10}H_{22}$ isomer	T
30B	143	$C_{10}H_{20}$ isomer	T
31	143	$C_{10}H_{22}$ isomer	0.15±0
32	146	*n*-propylbenzene + benzaldehyde	0.11±0
33	147	*m*-ethyltoluene	0.11±0
34	149	$C_{11}H_{24}$ isomer	0.12±0.1
35	151	$C_{11}H_{24}$ isomer	0.19±0.1
35A	153	C_3-alkyl benzene isomer	T
37	155	*n*-decane	0.15±0.1
38	159	$C_{11}H_{24}$ isomer	T
39	160	$C_{11}H_{24}$ isomer	T
39A	162	$C_{11}H_{22}$ isomer	T
40	163	$C_{12}H_{26}$ isomer	T
40A	164	acetophenone	T
41	170	$C_{12}H_{26}$ isomer	T
42	172	*n*-undecane	0.11±0
42A	180	$C_{10}H_{20}O$ isomer (tent.)	T
43A	184	2-decanone	T
43B	186	naphthalene	T
44	187	$C_{12}H_{24}$ isomer	T
45	188	*n*-dodecane	0.04±0
46A	197	C_4-alkyl benzene isomer	T
46B	199	undecanone isomer	T
47	201	undecanal (tent.)	T
47A	202	$C_{13}H_{26}$ isomer	T
48	203	*n*-tridecane	0.06±0
49A	216	$C_{14}H_{28}$ isomer	T
50	217	*n*-tetradecane	T
51A	220	$C_{16}H_{34}$ isomer	T
51B	221	$C_{15}H_{30}$ isomer	T
51C	226	$C_{15}H_{30}$ isomer	T

(continued)

Table C19 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb	Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
51D	229	$C_{16}H_{32}$ isomer	0.05±0			
52	230	$C_{15}H_{30}$ isomer	0.07±0			
53	231	*n*-pentadecane	0.04±			

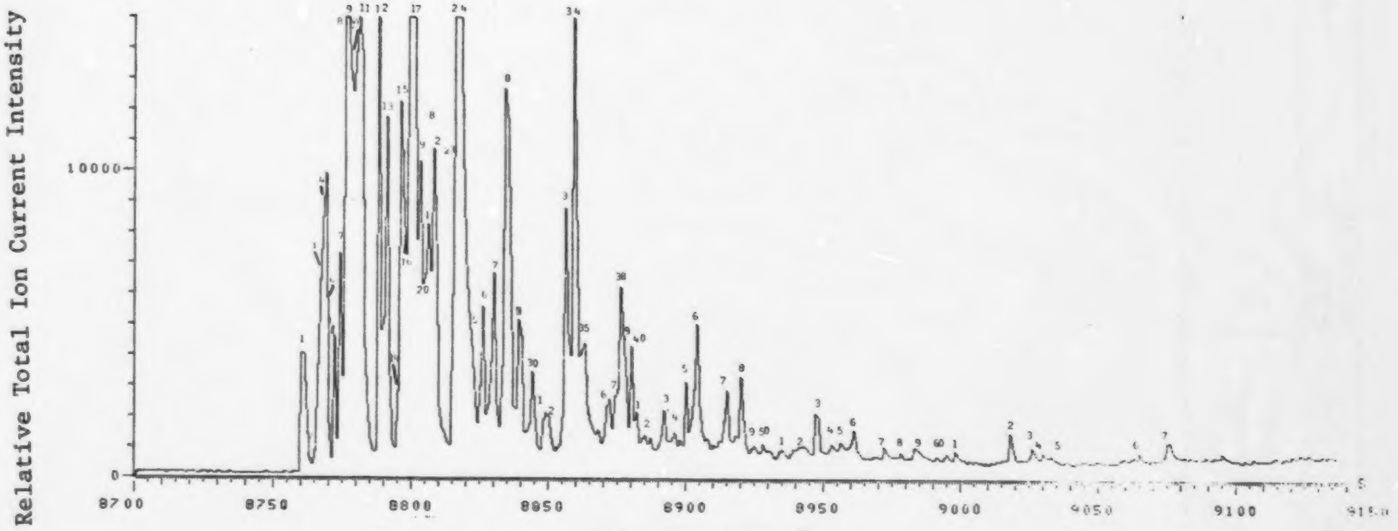


Figure C10. Profile of volatile organics in water sample (-9L) from environmental well #5 (LLL, ERDA).

Table C20. VOLATILE ORGANICS IN WATER SAMPLE (-9L) FROM ENVIRONMENTAL WELL #5 (LLL, ERDA)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
1	52	CO_2	NQ
2	55	n-propane	NQ
3	55	1-butene	NQ
4	56	n-butane	NQ
5	56	2-butene	NQ
6	58	trans-2-pentene	2.0±0.5
6A	59	acetaldehyde	1.2±0.3
7	59	isopentane	2.9±0.2
9	60	1-pentene	T
10	61	n-pentane	4.8±0.6
11	62	cis-2-pentene	0.6±0.1
11C	65	carbon disulfide + cyclopen-	-
		tadiene	0.2±0.1
12	66	cyclopentene	0.3±0
12A	67	C_6H_{12} isomer	T
13	67	cyclopentane	1.2±0.2
13A	68	2-methylpentane	5.4±0.5
13B	68	C_6H_{12} isomer	0.2±0
14	69	3-methylpentane	3.1±1.1
15	70	2-methylpent-1-ene	2.3±1.2
16	70	hexafluorobenzene (eF)	
17	71	n-hexane	6.0±3
18	72	2-methyl-2-pentene	0.5±0.1
19	73	hexadiene isomer	3.9±2.1
20	74	2-ethyl-1-butene	2.0±1
21	75	perfluorotoluene (eF)	
22	76	methylcyclopentane	4.8±2.1
22A	76	C_6H_{12} isomer	0.05±0
22B	77	methylcyclopentadiene isomer	4.4±2.1
22C	78	C_6H_{12} isomer	T
22D	79	C_7H_{12} isomer	T
23	80	methylcyclopentene isomer	5.9±2.5
24	80	benzene	10.6±3.2
24A	81	thiophene + C_7H_{14} isomer	0.8±0.2
24B	82	cyclohexane	0.8±0.3
24C	82	C_7H_{14} + C_7H_{12} isomer	0.2±0
25	83	2-methylhexane	0.4±0.1
25A	83	2,3-dimethylpentane	0.3±0.2
25B	84	3-methylhexane	0.4±0.1
26	85	cyclohexene	1.9±0.3
26A	85	C_7H_{14} isomer	0.05±0
26C	87	1,1-dimethylcyclopentane	0.6±0.3
27	87	1,2-dimethylcyclopentane	1.5±0.2
27A	88	5-ethyl-2-pentene	0.5±0.2
27B	89	heptene isomer	T
28	89	n-heptane	2.1±0.7
28A	90	methylhexadiene isomer	3.9±0.9
28B	90	trans-2-heptene	0.2±0.1
28C	91	methylhexene isomer	T
29	92	methylhexadiene isomer	2.2±0.3
29A	92	C_7H_{14} isomer	T
29B	93	C_7H_{12} isomer	T
30	94	methylcyclohexane	0.7±0.3
30A	95	dimethylhexadiene isomer	0.02±0
31	96	ethylcyclopentane	0.2±0.1
32	97	1-methylcyclohexene	0.4±0
32A	98	hexanal + C_8H_{16} isomer	T
32B	99	C_8H_{12} isomer	T
32C	99	2,3-dimethylhexa-1,4-diene	0.2±0
32D	100	2-methyl-2,4-hexadiene	4.4±1.3
33	101	C_8H_{14} isomer	T
33A	101	C_8H_{16} isomer	T
34	102	toluene	10±1
34A	102	C_8H_{14} isomer	T
34B	103	C_8H_{16} isomer	0.1±0
34C	103	C_8H_{18} isomer	T
35	104	methylcyclohexene isomer	0.8±0.3
35A	104	C_8H_{16} isomer	T
35B	105	3-methylheptane	T
35C	106	C_8H_{16} isomer	T
35D	106	C_8H_{14} isomer	T
35E	107	dimethylcyclohexane isomer	0.08±0
36	108	1,1,3-trimethylcyclopentane	0.2±0.1
36A	108	octene isomer	T
37	109	dimethylhexadiene isomer	0.07±0
37A	110	C_8H_{16} isomer	T
38	110	n-octane	0.2±0
39	111	C_8H_{16} isomer	T
39A	112	ethylidenecyclohexane	0.4±0.1
40	112	C_8H_{14} isomer	T
40A	113	C_8H_{16} isomer	T
41	114	C_9H_{18} isomer	T
41A	114	2-methyl-1,4-heptadiene	T
42	115	C_9H_{16} isomer	T
42A	116	C_8H_{14} isomer	T
42B	117	C_9H_{20} isomer	T
42C	118	C_3-alkyl cyclopentane isomer	T
43	118	C_8H_{14} isomer	T
43A	119	1,1,3-trimethylcyclohexane	0.3±0.1
43B	120	C_9H_{16} isomer	T
44	120	C_8H_{14} isomer	T

(continued)

Table C20 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
44A	121	C_9H_{18} isomer	T
44B	121	C_9H_{16} isomer	T
44C	122	C_9H_{18} isomer	T
45	122	ethylbenzene	0.5±0.1
45A	123	C_9H_{20} isomer + 3,3,5-trimethylcyclohexene	0.6±0.2
46	124	*m* or *p*-xylene	1.7±0.3
46A	125	C_9H_{18} isomer	T
46B	126	C_9H_{16} isomer	T
46C	126	C_9H_{20} isomer	T
46D	127	C_9H_{16} isomer	T
46E	128	C_9H_{18} isomer	T
46F	128	styrene + C_9H_{20} isomer	0.2±0
47	129	*o*-xylene	0.5±0.1
47A	130	C_9H_{18} isomer	0.05±0
47B	130	C_9H_{16} isomer	T
47C	131	C_9H_{18} isomer	T
48	132	*n*-nonane	0.8±0.2
48A	133	C_9H_{18} isomer	0.1±0
48B	134	C_9H_{16} isomer	0.05±0
49	135	C_9H_{18} isomer	T
49A	135	$C_{10}H_{20}$ isomer	T
50	136	$C_{10}H_{22}$ isomer	0.05±0
50A	137	$C_{10}H_{18}$ + C_9H_{16} isomers	T
50B	138	$C_{10}H_{20}$ isomer	T
50C	139	C_3-alkyl cyclohexane isomer	T
51	140	$C_{10}H_{22}$ isomer	T
51A	140	$C_{10}H_{18}$ isomer	T
51B	141	$C_{10}H_{22}$ isomer	T
51C	142	$C_{10}H_{18}$ isomer	T
51C	142	*n*-propylbenzene	T
51D	143	benzaldehyde	0.4±0.1
52	144	*m* or *p*-ethyltoluene	0.06±0
53	146	$C_{11}H_{24}$ isomer	0.2±0.1
54	149	$C_{11}H_{24}$ isomer	0.05±0
54A	149	2-octanone	T
54B	150	$C_{10}H_{22}$ isomer	T
55	151	C_3-alkyl benzene isomer	T
55A	152	$C_{10}H_{20}$ isomer	T
55C	153	$C_{10}H_{18}$ isomer	T
56	154	*n*-decane	0.2±0
56B	155	$C_{11}H_{22}$ isomer	T
56C	156	$C_{10}H_{20}$ isomer	T
56D	157	C_3-alkyl benzene isomer	T
56E	158		T
56F	158	$C_{11}H_{24}$ isomer	T
56G	159	$C_{11}H_{22}$ isomer	T
57	160	$C_{11}H_{24}$ isomer	0.05±0.01
58	163	$C_{12}H_{26}$ isomer	0.07±0.01
59	165	acetophenone	0.3±0.1
59A	166	$C_{12}H_{26}$ isomer	T
59B	167	$C_{11}H_{20}$ isomer	T
59C	168	$C_{11}H_{24}$ isomer	T
59D	168	$C_{11}H_{22}$ isomer	T
59E	169	2-nonanone	T
60	171	$C_{11}H_{22}$ isomer	T
60A	172	$C_{11}H_{20}$ isomer	T
61	172	*n*-undecane	0.1±0
61A	181	dimethylphenol isomer	NQ
62A	185	dimethylphenol isomer	NQ
63	187	naphthalene	0.04±0.02
63A	188	2-decanone	0.03±0.01
64	190	$C_{12}H_{24}$ isomer	T
65	191	*n*-dodecane	0.09±0.02
65A	207	$C_{13}H_{26}$ isomer	T
66	208	*n*-tridecane	0.13±0.06
66A	212	dimethylnaphthalene isomer	T

Table C21. VOLATILE ORGANICS IN WATER (-10L) FROM DEWATERING WELL #5 (LLL, ERDA)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb[a]
2	51	CO_2	NQ
3	55	1-butene	NQ
3A	56	n-butane	NQ
3B	56	2-butene	NQ
4	57	methanethiol	21.67
5A	61	acetone + C_5H_{10} isomer	750
5B	62	acetonitrile	19
5C	63	dimethyl sulfide	22
5D	63	C_5H_{10} isomer	0.5
5E	64	ter-butanol (tent.)	2.8
7	66	cyclopentene	5.8
7A	67	C_5H_{10} isomer	T
8	67	C_6H_{12} isomer	T
9	69	2-methylpentene	T
10	70	propionitrile	18.7
10A	70	methyl ethyl ketone	107
10B	71	n-hexane + hexafluorobenzene (eS)	140
10C	73	2-thiabutane	6.8
11	75	isobutyronitrile	4.0
12	76	methylcyclopentane	7.8
13	77	pentanol isomer	0.5
14	80	perfluorotoluene (eS)	
14A	81	3-methylcyclopentene	6.7
15	82	benzene	363
15A	83	3-methyl-2-butanone	20.8
15B	84	thiophene	28
15C	85	$C_4H_{10}S$ isomer (tent.)	NQ
15D	87	$C_6H_{14}O$ isomer	2.1
16	88	2-pentanone	90
17	90	3-pentanone	2.5
18	92	C_7H_{12} isomer	1.0
18A	93	$C_6H_{12}O$ isomer	T
19	93	2-thiapentane	0.9
19A	94	2,5-dimethylfuran (tent.)	0.7
20	95	C_7H_{14} isomer (tent.)	T
22	98	N-methylpyrrole	1.8
23	99	2,3-dithiabutane	0.2
23A	99	4-methyl-2-pentanone	30.2
24	102	2-methyl-3-pentanone	1.9
25	103	3-methyl-2-pentanone	0.9
25A	104	pyrrole	2.0
26	105	toluene	240
26A	106	n-pentylnitrile	13.6
26B	107	2-methylthiophene	150
26C	108	3-methylthiophene	170
27	109	3-hexanone	1.5
28	110	cyclopentanone	10.7
28A	111	2-hexanone	1.5
28C	114	C_8H_{14} isomer	T
29	115	thiacyclopentane	19.8
30	116	C_8H_{16} isomer	T
31	117	C_8H_{14} isomer	T
32	118	1-acetoxy-2-butene (tent.)	0.4
33A	119	2-amino-4-picoline (tent.)	59.5
33B	119	methylpyridine isomer	T
34	120	2-methylcyclopentanone	11.3
34A	121	$C_7H_{14}O$ isomer	T
35	121	3-methylcyclopentanone	7.8
36	122	2-methylthiacyclopentane +	15
		2-acetoxy-2-butene (tent.)	0.9
37	124	5-methyl-2-hexanone	5.9
38	125	ethylbenzene	12.5
38A	126	m-xylene	17.3
38B	126	ethylthiophene isomer	14.5
39	127	n-hexylnitrile	7.5
40	128	p-xylene	120
41	129	dimethylthiophene	20.9
42	130	3-heptanone	14.5
42A	131	dimethylthiophene isomer	6.9
43	132	2-heptanone	29.7
43A	132	styrene	6.7
43B	133	trimethylcyclopentane isomer	2.7
44	133	o-xylene	115
45	135	trimethylcyclohexane isomer	2.08
46	136	anisole	15.0
47	138	p-toluidine	4.8
47A	138	$C_8H_{16}O$ isomer	T
47B	139	C_3-alkyl thiophene isomer	0.15
48	139	isopropylbenzene + methyl cyclopentenyl ketone	6.1
48A	140	ethylpyridine isomer	4.1
49	141	C_9H_{18} + C_9H_{20} isomers	1.0
49A	141	C_9H_{16} isomer	T
50	143	2-methylcyclohexanone	0.3
51	144	1-methyl-3-ethylcyclopentane	2.6
52	145	n-propylbenzene	1.3
52A	146	2-isopropylthiophene	4.3
53	147	m-ethyltoluene	10.7
53A	148	p-ethyltoluene + C_3-alkyl thiophene isomer	6.2

(continued)

Table C21 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
54	149	1,3,5-trimethylbenzene + $C_{11}H_{24}$ isomer	3.3
54A	150	cyanobenzene	5.5
55	152	2-octanone	2.0
56	153	C_3-alkyl thiophene isomer	T
57	154	benzofuran	91.7
57A	154	o-ethyltoluene	19.4
57C	156	phenol	NQ
57D	157	$C_{10}H_{20}$ isomer	T
58	158	p-methylanisole	5.5
58A	159	1,2,4-trimethylbenzene + C_4-alkyl benzene isomer	19.4
59	160	C_4-alkyl benzene isomer	110
60	161	trimethylcyclohexanone isomer (tent.)	1.87
61	162	indan	55.2
62	163	indene	22.2
62A	165	C_4-alkyl benzene isomer	1.5
62B	165	trimethylcyclohexanone isomer	NQ
63	166	acetophenone	
63A	166	ter-butylthiophene isomer	2.5
64	167	p-cresol	NQ
65	168	C_4-alkyl benzene isomer	90
66	168	m-cresol	NQ
67	170	C_4-alkyl benzene isomer	T
67A	170	2-nonanone	16.7
68	171	C_4-alkyl benzene isomer	T
69	171	methylindan isomer	2.89
70	172	C_4-alkyl benzene isomer	0.1
71	173	2-methylbenzimidazole	6.81
72	174	dimethylphenol isomer	NQ
72A	175	methylbenzimidazole isomer	72.9
73	176	C_5-alkyl benzene + $C_{11}H_{20}$ isomers	T
74	176	$C_{11}H_{22}$ isomer	T
74A	177	C_4-alkyl benzene isomer	T
75	178	tetramethylbenzene isomer	T
76	179	C_4-alkyl benzene isomer	T
77	180	C_5-alkyl benzene isomer	T
78	181	methylindan isomer	6.0
78A	181	C_5-alkyl benzene isomer	T
78B	182	$C_{11}H_{20}$ isomer	T
79	183	methylindene isomer	4.0
79A	183	$C_{10}H_{12}$ isomer	T
80	184	C_4-alkyl benzene isomer	0.15
80A	184	methylindene isomer	3.2
80B	185	dimethylphenol isomer	NQ
81	185	C_5-alkyl benzene isomer	T
82	187	C_4-alkyl benzene isomer	T
82A	188	$C_{11}H_{20}$ isomer	T
82B	189	C_3-alkyl phenol isomer	NQ
83	190	naphthalene	74.7
83A	193	thianaphthalene + dimethylindan isomer	22.5 7.2
84	194	5,6-dimethylbenzofuran	15.5
85	195	3,6-dimethylbenzofuran	7.6
86	196	C_5-alkyl benzene isomer	T
87	199	C_5-alkyl benzene isomer	T
88	200	$C_{12}H_{22}$ isomer	T
89	201	$C_{11}H_{14}$ isomer	T
90	202	methyldihydronaphthalene isomer	4.3
91	203	$C_{12}H_{16}$ isomer	T
92	204	6-methyl-1,2-dihydronaphthalene	5.1
93	205	C_7-alkyl benzene isomer	T
94	206	C_3-alkyl indan isomer	T
95	207	dimethylindan isomer	1.7
96	208	C_3-alkyl indan isomer	1.5
97	209	β-methylnaphthalene	11.7
98	210	C_3-alkyl indan isomer	3.0
99	212	α-methylnaphthalene	2.0
99A	212	C_4-alkyl indan isomer	T
100	213	C_3-alkyl indan isomer	T
102	224	$C_{16}H_{34}$ isomer	T
103	239	$C_{17}H_{36}$ isomer	T

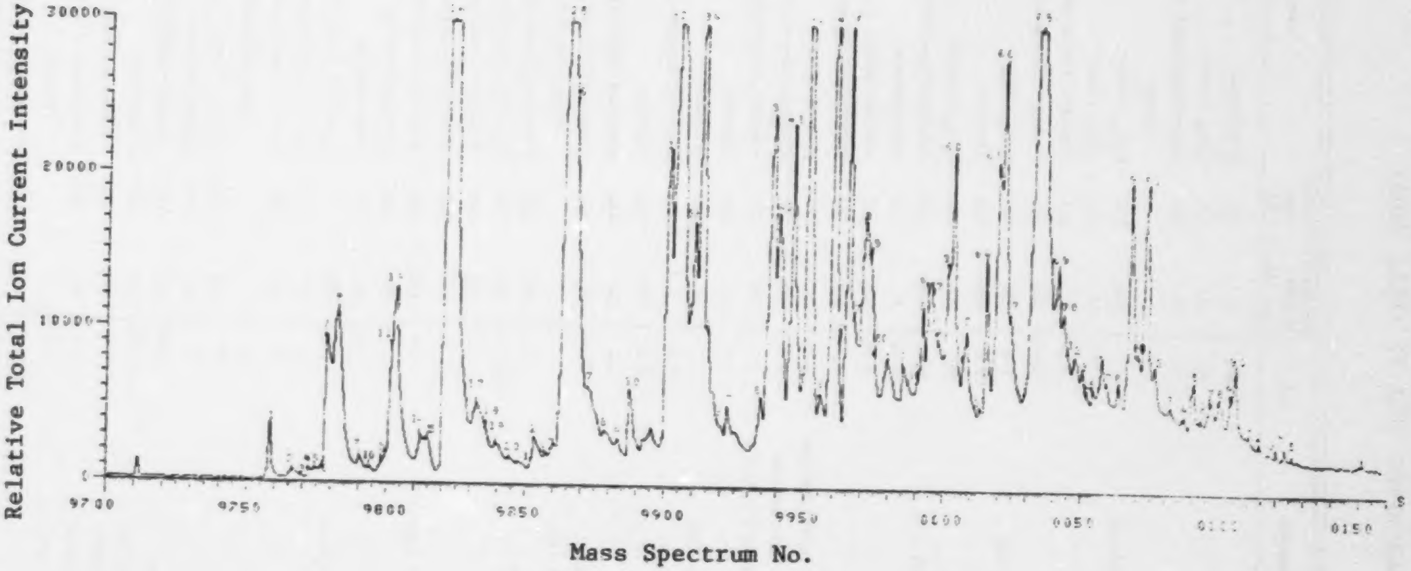


Figure C11. Profile of volatile organics in water sample (-11L) from dewatering well #5 (LLL, ERDA).

Table C22. VOLATILE ORGANICS IN WATER (-11L) FROM DEWATERING WELL #5 (LLL, ERDA)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb[a]	Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
1	50	CO_2	NQ	27	107	2-hexanone	55.4
1A	54	1-butene	NQ	27A	109	C_8H_{16} isomer	T
2	54	n-butane	NQ	28	110	thiacyclopentane + C_8H_{14} isomer	0.59
3	55	2-butene	NQ	28A	111	C_8H_{16} isomer	T
4	57	methanethiol + unknown	T	29	113	C_8H_{14} isomer	T
4A	58	C_5H_{10} isomer	T	30A	116	5-methyl-3-hexanone	2.04
5	58	acetaldehyde	3.57	30B	117	2-methyl-3-hexanone	T
5A	59	isopentane	0.90	30C	117	C_9H_{20} isomer	T
6	60	C_5H_{10} isomer + furan	5.0	30D	118	pyridine	1.71
7	61	acetone	47.6	30E	118	$C_7H_{14}O$ isomer	T
7A	62	dimethyl sulfide	NQ	30F	119	2-methylthiacyclopentane	0.94
8B	64	C_3H_8S isomer (tent.)	NQ	31	121	ethylbenzene	34.3
8C	65	ter-butanol	4.28	31A	122	ethylthiophene isomer	9.32
9	66	cyclopentene	5.38	31B	123	dimethylthiophene isomer	16.6
9A	67	cyclopentane	0.72	32	124	p or m-xylene	621.7
10	68	C_6H_{12} isomer + 2-methylpentane	0.71	32A	125	dimethylthiophene isomer	41.4
11	70	propionitrile + 2-thiapentane (tent.) + 3-methylpentane	2.55	32B	127	dimethylthiophene isomer	12.4
11A	71	C_6H_{12} isomer	T	33	128	styrene	13.3
12	71	hexafluorobenzene (eS)		34	129	o-xylene	32.4
12A	72	methyl ethyl ketone	21.4	35	131	dimethylthiophene isomer	7.59
13	73	n-hexane	18.8	35A	132	anisole	T
13B	76	C_6H_{12} isomer	T	36	133	dimethylthiophene isomer	T
14	77	methylcyclopentane	2.54	37	134	isopropylbenzene + isopropyl-thiophene isomer	1.91 1.43
15	79	perfluorotoluene (eS)		37A	135	2-methyl-3-heptanone	0.82
15A	81	C_6H_{10} isomer	T	37B	136	C_3-alkyl thiophene isomer	T
16	82	benzene	158.9	37C	137	5-methyl-3-heptanone	2.50
16A	83	thiophene	41.4	37D	138	6-methyl-3-heptanone	1.19
16B	87	cyclohexene	1.43	37E	139	5-methyl-2-heptanone	5.35
17	87	methyl isopropyl ketone	7.62	38	140	n-propylbenzene	2.86
17A	88	C_7H_{14} isomer	T	38A	141	benzaldehyde	8.98
18	89	3-pentanone	7.43	38B	141	C_3-alkyl thiophene isomer	T
19	91	C_7H_{12} + C_7H_{16} isomers	T	39	142	m or p-ethyltoluene	32.4
19A	92	C_7H_{14} isomer	T	40	143	1,3,5-trimethylbenzene + C_3-alkyl thiophene isomer	33.1
20	93	C_7H_{12} isomer	T	40A	144	$C_{10}H_{22}$ isomer	T
20A	94	C_7H_{14} isomer	T	41	145	o-ethyltoluene	27.6
20B	95	C_7H_{12} isomer	T	41A	146	trimethylthiophene isomer	8.3
21	95	C_7H_{14} isomer	T	41B	147	2-octanone	T
21A	97	2,3-dithiabutane	2.86	41C	148	α-methylstyrene	T
22	98	4-methyl-2-pentanone	2.32	42	149	benzofuran + 1,2,4-trimethyl-benzene	119.0 26.7
23	100	2-methyl-3-pentanone	9.76	43	151	trimethylthiophene isomer	14.0
24	101	3-methyl-2-pentanone	4.57	43A	151	ter-butylthiophene isomer	3.67
24A	101	methylhexadiene isomer	1.60	43B	152	isobutylbenzene	T
25	102	toluene	219.0				
26	105	2-methylthiophene	40.0				
26A	106	3-hexanone	5.89				

(continued)

Table C22 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
44	152	1,2,3-trimethylbenzene	33.1
45	153	C_4-alkyl benzene isomer	T
45A	154	C_4-alkyl thiophene isomer	T
46	156	indan	54.1
47	157	C_4-alkyl benzene isomer	T
48	158	indene	T
49	159	C_4-alkyl benzene isomer	16.2
49A	160	C_4-alkyl thiophene isomer	T
50	161	C_4-alkyl benzene isomer	T
50A	161	C_8H_8O isomer (tent.)	NQ
50B	162	*p*-propyltoluene + C_4-alkyl thiophene isomer	2.50 1.21
51	163	*o*-diethylbenzene + *n*-butylbenzene	3.05 3.05
51A	164	C_4-alkyl thiophene isomer	5.15
52	166	C_4-alkyl benzene isomer	T
52A	166	C_8H_8O isomer (tent.)	NQ
53	167	C_4-alkyl thiophene isomer	1.72
54	168	C_4-alkyl benzene isomer	T
54A	169	methylindan isomer	T
55	169	C_4-alkyl benzene isomer	T
55A	170	$C_{10}H_{12}$ isomer + methylindene	3.35
56	171	dimethylethylbenzene isomer	6.97
57	172	methylindan isomer	6.19
57A	172	C_4-alkyl thiophene isomer	T
58	173	C_4-alkyl benzene isomer	T
58A	173	$C_{10}H_{12}$ isomer	T
58B	174	*o*-cresol	NQ
59	174	methylbenzofuran isomer	10.0
60	175	2-methylbenzofuran	27.4
60A	175	C_4-alkyl benzene isomer	T
60B	176	C_5-alkyl benzene isomer	T
61	177	C_4-alkyl benzene + C_4-alkyl thiophene isomers	4.25
62	178	tetramethylbenzene isomer	7.62
62A	178	C_5-alkyl thiophene isomer	T
63	180	C_5-alkyl benzene isomer	T
63A	181	$C_{11}H_{14}$ isomer	T
64	181	$C_{10}H_{12}$ isomer	10.5
64A	182	C_5-alkyl benzene isomer	T
64B	182	dimethylphenol + C_5-alkyl thiophene isomers	NQ
65	183	methylindene isomer	T
65A	183	methylindan isomer	13.1
66	184	tetramethylbenzene + methylindene isomers	14.3 18.1
67	185	C_5-alkyl benzene isomer	15.3
67A	186	dimethylphenol isomer	NQ
67B	187	tetramethylbenzene isomer	T
67C	188	dimethylphenol isomer	NQ
68	189	naphthalene	133.3
68A	191	dimethylindan isomer	T
68B	192	2,3-benzothiophene	4.30
68C	193	dimethylindan isomer	9.52
69	195	dimethylbenzofuran isomer	7.14
70	196	C_3-alkyl phenol isomer	NQ
71	197	$C_{11}H_{14}$ isomer	T
72	198	C_5-alkyl benzene + C_3-alkyl phenol isomers	15.2 NQ
72A	199	$C_{11}H_{14}$ isomer	T
73	200	methyldihydronaphthalene isomer	1.14
74	201	$C_{11}H_{14}$ isomer	T
75	202	methyldihydronaphthalene isomer .	3.20
75A	202	$C_{12}H_{16}$ isomer	T
76	203	methyldihydronaphthalene + C_4-alkyl phenol isomers	3.54 T
77	204	C_6-alkyl benzene isomer	25.3
77A	205	C_3-alkyl indan isomer	7.9
77B	206	C_4-alkyl phenol isomer	NQ
78	206	$C_{11}H_{14}$ isomer	T
78A	207	6-methylbenzo(b)thiophene	1.27
78B	207	C_3-alkyl indan isomer	T
79	208	β-methylnaphthalene	140.1
80	209	$C_{12}H_{16}$ isomer	T
80A	210	methylbenzothiophene isomer	0.41
81	211	α-methylnaphthalene	38.3
82	212	$C_{12}H_{16}$ isomer	T
82A	214	C_5-alkyl phenol isomer	NQ
83	215	$C_{12}H_{16}$ isomer	T
84	217	C_4-alkyl indan isomer	T
85	219	biphenyl	6.07
86	220	$C_{12}H_{14}$ isomer	T
86A	221	C_4-alkyl indan isomer	T
87	223	ethylnaphthalene isomer	3.42
87A	224	$C_{13}H_{18}$ + $C_{12}H_{14}$ isomers	T
88	225	dimethylnaphthalene isomer	4.86
88A	226	$C_{13}H_{18}$ isomer	T
89	227	dimethylnaphthalene isomer	5.71
90	228	dimethylnaphthalene isomer	4.49
91	230	dimethylnaphthalene isomer	T
92	232	C_2-alkyl naphthalene isomer	1.78
93	235	ethylnaphthalene isomer	T

[a] Values represent single determinations.

Table C23. VOLATILE ORGANICS IN WATER (-12L) FROM ENVIRONMENTAL MONITORING WELL #1, POST-GASIFICATION (LLL, ERDA)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
1	41	CO_2	-
4	44	propane	NQ
4A	44	acetaldehyde	T
5	45	1-butene + *n*-butane	NQ
5A	46	2-butene	NQ
6B	48	isopentane	0.37±0.1
7A	50	*n*-pentane	130.00±60
8	51	acetone	181.12±60
8A	51	dimethyl ether + diethyl ether	10±5
10	57	C_5H_{10} isomer	3.50±1.5
10A	58	2-methylpentane	2.60±1.8
11	59	3-methylpentane	5.75±1.3
12	61-7	*n*-hexane	
12A	62	hexafluorobenzene (eS)	
13A	67	perfluorotoluene (eS) + methylcyclopentane	25.00±12
13B	72	benzene	42.22±24
14	72	cyclohexane	NQ
16	79	C_7H_{16} isomer	90.00±40
17	91-5	toluene	40.00±30
17A	96	C_8H_{18} isomer	3.26±1.3
20	106	C_9H_{20} isomer	1.86±0.4
21	110	ethylbenzene	4.44±2.2
22	115	$C_{10}H_{22}$ isomer	T
23	116	$C_{10}H_{22}$ isomer	T
23A	117	styrene	7.78±1.3
24	118	$C_{10}H_{22}$ isomer	9.00±4.5
24A	120	$C_{10}H_{20}$ isomer	T
25	121	$C_{10}H_{22}$ isomer	3.20±1.4
26	122	$C_{10}H_{22}$ isomer	150.00±70
27	123	$C_{10}H_{20}$ isomer	3.50±2.0
28	124	$C_{10}H_{22}$ isomer	100.00±40
29	126	$C_{10}H_{20}$ isomer	T
30	129	$C_{11}H_{24}$ isomer	4.10±2.0
31	130	$C_{11}H_{24}$ isomer	130.05±60
32	133	$C_{11}H_{24}$ isomer	260.00±180
33	134	$C_{11}H_{24}$ isomer	170.00±100
34	136	$C_{11}H_{24}$ isomer	130.00±80
35	137	$C_{11}H_{22}$ isomer	90.00±50
36	139	$C_{11}H_{24}$ isomer	15.00±12
37	141	$C_{12}H_{26}$ isomer	7.60±3.8
38	143	$C_{12}H_{26}$ isomer (tent.)	7.50±2.0
39	144	$C_{13}H_{28}$ isomer (tent.)	2.00±1.0
40	147	$C_{13}H_{28}$ isomer	T
41	153	$C_{13}H_{26}$ isomer	T
42	163	naphthalene (tent.)	100±50
43	168	$C_{13}H_{26}$ + $C_{13}H_{28}$ isomers	T
44	181	methylnaphthalene isomer	168.88±60
45	184	methylnaphthalene isomer	111.00±70
46	186	$C_{12}H_{16}$ isomer	0.26±0.13
47	188	$C_{12}H_{16}$ isomer	T
48	189	$C_{12}H_{16}$ + $C_{13}H_{18}$ isomers	T
49	190	$C_{13}H_{18}$ isomer	T
50	192	$C_{14}H_{26}$ isomer (tent.)	2.80±1.2
51	193	$C_{14}H_{26}$ isomer	0.50±0.3
52	193	$C_{14}H_{30}$ isomer	0.60±0.3
53	194	$C_{14}H_{24}$ isomer (tent.)	1.20±0.3
53A	196	dimethylphenanthrene isomer	0.56±0.2
54	198	$C_{14}H_{30}$ isomer	2.60±1.3
55	203	dimethylphenanthrene isomer	0.44±0.2

Table C24. VOLATILE ORGANICS IN WATER (-13L) FROM ENVIRONMENTAL MONITORING WELL #4, POST-GASIFICATION (LLL, ERDA)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
2	42	CO_2	-
2A	44	acetaldehyde	T
2B	45	C_4H_8 isomer + *n*-butane	NQ
3	45	C_4H_8 isomer	T
3A	47	C_5H_{10} isomer	T
3B	48	C_5H_{12} isomer	T
3C	49	C_5H_{10} isomer	T
3D	50	C_5H_{10} isomer	T
4A	54	C_5H_8 isomer	T
4B	55	C_5H_{10} isomer	T
4C	57	diethyl ether (tent.)	0.13±0.1
5	60	C_6H_{14} isomer	0.17±0.1
6	63	perfluorobenzene (eS)	
6A	63	*n*-hexane	5.00±2.5
8	66	perfluorotoluene (eS)	
8A	67	C_6H_{12} isomer	T
9	69	benzene	290±90
9A	72	thiophene	0.87±0.3
9B	74	C_6H_{10} isomer	T
10A	82	C_7H_{14} isomer	T
10B	85	C_7H_{12} isomer	T
10C	87	C_7H_{12} isomer	T
10D	88	C_7H_{12} isomer	T
11	89	toluene	
11B	101	C_8H_{14} isomer	T
11C	103	C_8H_{14} isomer	T
11D	106	C_9H_{18} isomer	T
13	110	ethylbenzene + C_9H_{16} isomer	0.25±0.1
13A	112	xylene isomer	0.23±0.1
13B	114	C_9H_{20} isomer	0.16±0.1
13C	115	C_9H_{20} isomer	0.12±0.1
13D	115	xylene isomer	0.26±0.1
13E	117	C_9H_{20} isomer	0.15±0.1
13F	118	$C_{10}H_{22}$ isomer	0.12±0.1
13G	120	$C_{10}H_{22}$ isomer	0.09±0
14	129	$C_{11}H_{24}$ isomer	3.25±1
14A	129	C_3-alkyl benzene isomer	T
15	131	$C_{11}H_{24}$ isomer	0.50±0.3
16	135	$C_{10}H_{20}$ isomer	0.61±0.1
16A	135	benzaldehyde	0.30±0.1
16B	139	C_3-alkyl benzene + C_4-alkyl benzene isomers	T
16C	139	$C_{11}H_{22}$ isomer	T
16D	142	$C_{11}H_{24}$ isomer	T
16F	143	phenol	NQ
16G	144	$C_{11}H_{22}$ isomer	T
17	153	$C_{11}H_{24}$ isomer	T
17A	154	acetophenone	0.50±0.2
17B	155	$C_{10}H_{12}$ isomer (tent.)	T
17C	156	C_4-alkyl benzene isomer (tent)	T
17D	159	cresol isomer	NQ
17F	163	C_2-alkyl phenol isomer	NQ
18	167	naphthalene	0.53±0.1
19	169	C_2-alkyl phenol isomer	NQ
19A	169	*n*-dodecane	0.18±0.1
19B	177	C_4-alkyl phenol isomer	NQ
20	184	β-methylnaphthalene	0.47±0.2
20A	185	*n*-tridecane	0.22±0.1
21	186	α-methylnaphthalene	0.74±0.3
22	188	$C_{12}H_{16}$ isomer	T
22A	189	$C_{13}H_{18}$ isomer	T
23	190	$C_{13}H_{18}$ + 1-phenylheptane	0.42±0.2
24	192	C_2-alkyl benzene isomer	1.28±0.7
25	193	$C_{13}H_{18}$ isomer	T
26	195	biphenyl	6.20±4.0
27	196	$C_{15}H_{32}$ isomer	2.10±1.0
27A	197	$C_{14}H_{28}$ + $C_{13}H_{14}$ isomers	1.70±0.1
27B	198	C_2-alkyl naphthalene isomer	T
27C	198	$C_{14}H_{30}$ isomer	T
27D	199	$C_{15}H_{30}$ isomer	T
28	200	$C_{14}H_{20}$ isomer	T
29	203	2,4-ditertiary butyl phenol	NQ
31	205	$C_{15}H_{26}$ isomer (tent.)	T
32	206	unknown	NQ
34	244	*n*-$C_{17}H_{32}$ isomer	T

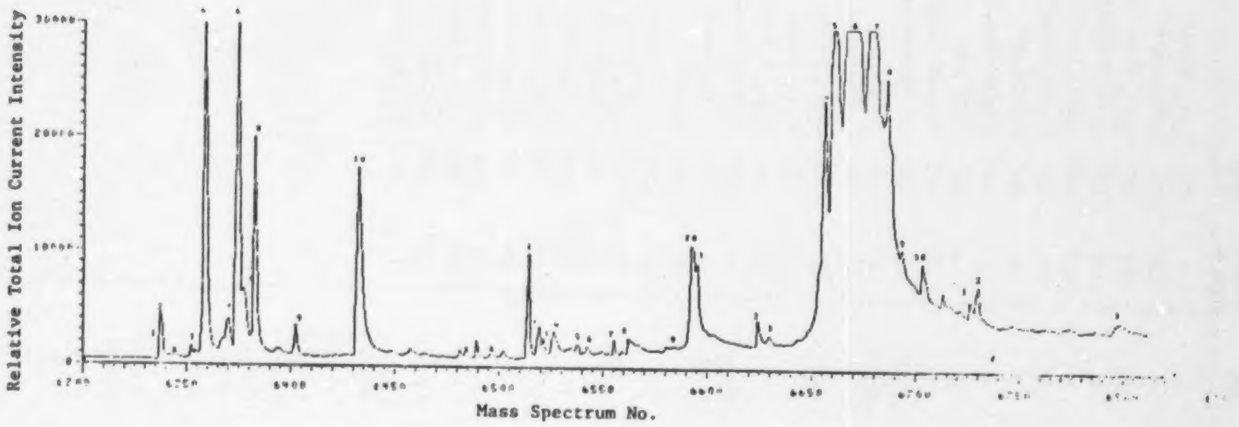


Figure C12. Profile of volatile organics in water sample (-14L) from environmental monitoring well #2, post-gasification (LLL, ERDA).

Reproduced from best available copy.

Table C25. VOLATILE ORGANICS IN WATER (-14L) FROM ENVIRONMENTAL MONITORING WELL #2, POST-GASIFICATION (LLL, ERDA)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
2	39	CO_2	-
2B	41	C_4H_8 isomer	NQ
2C	42	C_4H_8 + C_4H_{10} isomers	NQ
2D	43	C_4H_8 isomer	T
2E	43	acetaldehyde	T
2F	44	C_5H_{10} isomer	T
2G	45	C_5H_{12} isomer	T
3A	48	C_5H_{12} isomer	T
3B	48	furan + C_5H_{10} isomer	0.89±0.3
4A	52	propanal	T
4B	53	diethyl ether	T
4C	53	C_5H_{10} isomer	T
4D	54	C_6H_{14} isomer + unknown	NQ
5	55	acetone	0.87±0.3
5A	56	C_6H_{14} isomer	1.20±0.6
6	57	perfluorobenzene (eS)	
6A	58	*n*-hexane	9.17±3.9
7A	61	C_7H_{16} isomer	0.03±0
8	61	perfluorotoluene (eS)	
8A	62	C_6H_{12} isomer	T
8B	64	C_7H_{14} isomer + *n*-butanal (tent.)	T
8C	64	C_7H_{14} isomer (tent.)	T
8D	67	benzene	0.22±0.1
8F	68	C_7H_{16} isomer	T
9A	74	C_7H_{14} isomer	T
10	86	toluene	43.34±10
10A	94	*n*-octane	T
10B	106	ethylbenzene	T
10C	108	xylene isomer	0.83±0.4
10D	111	C_9H_{20} isomer	0.25±0.2
10E	113	styrene + C_2-alkyl benzene isomer	T
10F	114	*n*-nonane	0.37±0.2
10G	117	$C_{10}H_{22}$ isomer	0.25±0.1
10H	121	$C_{10}H_{22}$ isomer	0.13±0
10I	125	$C_{10}H_{22}$ isomer	T
10J	126	C_3-alkyl benzene isomer	T
11	126	$C_{11}H_{24}$ isomer	4.00±3.2
12	129	$C_{11}H_{24}$ isomer	0.60±0.3
13	130	$C_{11}H_{24}$ isomer	0.57±0.3
13A	131	C_3-alkyl benzene isomer	T
14	132	$C_{10}H_{22}$ isomer	0.75±0.1
14A	133	$C_{10}H_{22}$ isomer	0.60±0.1
14B	134	benzaldehyde	0.28±0.1
14C	137	C_3-alkyl benzene isomer	0.35±0.1
15	138	$C_{11}H_{24}$ isomer	0.26±0.1
16	141	$C_{12}H_{26}$ isomer	T
16A	144	phenol + C_4-alkyl benzene isomer	NQ
16B	146	C_5-alkyl benzene isomer	T
17A	149	$C_{11}H_{22}$ isomer	T
18	150	*n*-undecane	T
18A	151	acetophenone + methylbenzofuran isomer	0.85±0.1
18B	155	cresol isomer	NQ
18C	158	cresol isomer	NQ
18D	149	C_4-alkyl benzene + C_5-alkyl benzene isomers	NQ
18E	160	cresol isomer (tent.)	NQ
19	160	C_2-alkyl phenol isomer	NQ
19A	163	C_2-alkyl phenol isomer	NQ
20	165	naphthalene	94.44±38.8
20A	167	*n*-dodecane	1.11±0.5
21	167	C_2-alkyl phenol isomer	NQ
21A	169	C_2-alkyl phenol + C_2-alkyl benzofuran isomers	NQ
21B	170	C_3-alkyl phenol isomer	NQ
21C	177	$C_{13}H_{28}$ isomer	NQ
21D	178	C_3-alkyl phenol isomer	NQ
22	182	β-methylnaphthalene	0.35±0.2
23	184	α-methylnaphthalene	0.50±0.2
23A	193	biphenyl	0.13±0.1
23B	195	ethylnaphthalene + C_3-alkyl tetrahydronaphthalene isomers	0.36±0.2
24	197	dimethylnaphthalene isomer	4.71±2.1
25	199	C_2-alkyl naphthalene isomer	T
25A	200	$C_{13}H_{18}$ isomer	T
26	205	C_2-alkyl naphthalene + $C_{14}H_{20}$ (tent.) isomers	T
26A	206	biphenylene	8.33±2.6
26B	207	C_2-alkyl naphthalene isomer	2.80±1.4
26C	207	$C_{16}H_{34}$ isomer	T
26D	208	C_2-alkyl naphthalene + $C_{14}H_{20}$ isomers	T
27	209	acenaphthene	4.68±0.4
27A	210	$C_{14}H_{20}$ isomer (tent.)	5.00±2.0
27B	211	*n*-pentadecane	T
27C	212	$C_{15}H_{30}$ isomer	T
27D	212	C_8-alkyl phenol or $C_{16}H_{14}$ isomers	NQ

(continued)

Table C25 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb	Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
30A	223	*n*-hexadecane	0.25±0.1			
32	240	$C_{17}H_{36}$ isomer	2.50±1.0			

Table C26. VOLATILE ORGANICS IN LIQUID SAMPLE (-15T) FROM PRODUCTION WELL #1, POST-GASIFICATION (LLL, ERDA)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppm
1	40	$N_2 + O_2$	-
2	41	CO_2	-
3	44	C_4H_8 isomer	NQ
5	48	acetaldehyde	24±10
8	53	diethyl ether	T
9	56	acetone	9.2±2.2
10	57	perfluorobenzene (eS)	
11	58	C_6H_{14} isomer	T
13	62	perfluorotoluene (eS)	
14	88	toluene	31.2±14
15	91	C_8H_{16} isomer	5.2±1
16	92	C_8H_{18} isomer	6.2±1.4
18	113	C_2-alkyl benzene isomer	2±0.6
19	113	styrene	T
20	115	C_9H_{20} isomer	T
21	126	C_3-alkyl benzene isomer	T
22	128	$C_{10}H_{22}$ isomer	1±0.7
23	132	C_3-alkyl benzene isomer	5.6±0.4
24	133	benzaldehyde	6±2
26	134	benzofuran	2±1
27	134	$C_{10}H_{22}$ isomer	2.8±1.2
28	137	C_4-alkyl benzene isomer	1.6±0.4
29	138	phenol	NQ
30	139	C_4-alkyl benzene isomer	3.2±1.6
31	142	C_4-alkyl benzene isomer	5.6±1
32	145	C_4-alkyl benzene isomer	5.7±0
33	149	C_4H_7-benzene isomer	T
34	150	C_4H_7-benzene isomer	T
35	150	$C_{11}H_{22}$ isomer	1±0.9
36	151	methylbenzofuran isomer	6.6±2.4
37	152	dioxan (tent.)	24±10
38	152	$C_{11}H_{24}$ isomer	T
39	153	methylbenzofuran isomer	6±2.2
40	155	ethylphenol isomer	NQ
41	157	C_5-alkyl benzene isomer	T
42	158	ethylphenol isomer	NQ
43	160	ethylphenol isomer	NQ
44	160	C_5-alkyl benzene isomer	8.8±3
45	165	naphthalene	12.4±3
46	166	$C_{12}H_{24}$ isomer	T
47	166	C_4-alkyl benzene isomer	T
48	167	C_5H_{10}-benzene isomer	0.2±0
49	168	$C_{12}H_{26}$ isomer	3.2±0.2
50	169	C_5H_9-benzene isomer	16.4±2
51	170	C_6H_{11}-benzene isomer	T
52	171	dimethylbenzofuran isomer	0.6±0.4
53	173	$C_{12}H_{22}$ isomer	T
54	178	C_6H_{11}-benzene isomer	T
55	181	trimethylindan isomer	T
56	182	β-methylnaphthalene	8±2
57	184	C_6H_{11}-benzene isomer	T
58	185	α-methylnaphthalene	24±2.1
59	187	C_6H_{11}-benzene isomer	T
60	192	C_6H_{11}-benzene isomer	T
61	195	$C_{13}H_{26}$ isomer	T

Table C27. VOLATILE ORGANICS IN WATER (-16L) FROM DEWATERING WELL #4, POST-GASIFICATION (LLL, ERDA)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
1	41	CO_2	-
2	44	C_4H_8 isomer + n-butane	NQ
2A	44	acetaldehyde	T
3	45	C_4H_8 isomer	T
3A	47	isopentane	T
3B	49	C_5H_{10} isomer	0.25±0
3C	49	n-pentane	0.44±0.1
4	50	furan	0.19±0
4A	50	C_5H_{10} + C_2H_6S isomers	T
5	51	acetone	9.52±1.7
5A	52	carbon disulfide (tent.)	NQ
5B	54	C_5H_8 isomer	T
5C	58	C_6H_{14} isomer	T
5D	58	C_6H_{12} isomer	T
5E	58	2-propanol	0.95±0.1
6	60	perfluorobenzene (eS)	
6A	60	n-hexane	0.16±0
6B	61	C_6H_{12} isomer	T
7A	62	propionitrile	3.20±1.1
7B	64	methyl ethyl ketone	1.78±0.8
8	64	perfluorotoluene (eS)	
9	68	benzene + C_6H_{10} isomer + isobutyronitrile	97.73±17
9A	70	thiophene	5.63±0.5
10	73	methyl isopropyl ketone	1.18±0.3
11	76	C_7H_{12} isomer	T
11A	80	C_7H_{12} + C_7H_{14} isomers	T
11B	81	n-butyronitrile	2.40±1.0
12	81	C_7H_{12} isomer	T
12A	82	2-pentanone	2.51±0.6
12B	84	3-pentanone	0.56±0.1
12C	86	C_7H_{12} isomer	T
12D	88	α-methylbutyronitrile	T
13	88	C_7H_{12} isomer + 4-methyl-2-pentanone	2.75±0.9
13A	88	2-methyl-3-pentanone	5.14±1.0
13B	88	3-methyl-2-pentanone	3.25±0.6
14	89	toluene	5.38±0.8
14A	89	methylthiophene isomer	6.75±0.6
15	91	methylthiophene isomer	6.77±0.5
15A	96	C_8H_{14} isomer	T
15B	97	acetic acid (tent.)	NQ
15C	98	C_8H_{14} isomer	T
15D	100	3-hexanone	0.34±0.2
15E	101	2-hexanone	0.41±0.1
15F	101	C_8H_{14} isomer + cyclopentanone	T
15G	103	$C_7H_{14}O$ ketone isomer	0.11±0
16	104	$C_7H_{14}O$ ketone isomer	1.92±0.5
16A	105	$C_5H_{10}S$ isomer	T
16B	105	$C_6H_{10}O$ isomer	T
17	108	ethylbenzene	33.25±7.0
18	109	C_2-alkyl thiophene isomer	0.88±0.1
18A	110	xylene + C_2-alkyl thiophene isomers	68.57±13
19	111	C_2-alkyl thiophene isomer	T
20	113	C_2-alkyl thiophene isomer	0.55±0.1
20A	113	styrene	3.73±1.0
21	114	xylene isomer	60.00±10
22	117	C_2-alkyl thiophene isomer	T
23	119	C_9H_{18} isomer	T
24	121	isopropylbenzene + C_3-alkyl thiophene isomer	32.00±17
24A	123	C_3-alkyl thiophene isomer	T
25	124	$C_8H_{16}O$ ketone isomer	0.78±0.2
26	126	n-propylbenzene	34.00±4.0
27	127	C_3-alkyl benzene + C_3-alkyl thiophene isomers	2.50±1.2
28	129	C_3-alkyl thiophene isomer	1.08±0.3
29	131	C_3-alkyl benzene isomer	T
29A	131	C_3-alkyl thiophene isomer	T
30	134	C_3-alkyl benzene + benzofuran	T
31	137	C_3-alkyl thiophene isomer	T
31A	137	C_4-alkyl thiophene isomer	T
32	138	C_4-alkyl benzene isomer	5.81±1.1
32A	139	C_3-alkyl benzene isomer	T
33	141	C_9H_{10} isomer or indan	0.88±0.2
34	143	C_9H_8 isomer or indene	1.10±0.5
35	144	C_4-alkyl benzene isomer	3.94±0.5
35A	144	C_4-alkyl thiophene isomer	T
36	145	C_4-alkyl benzene isomer	1.50±0.5
37	146	C_4-alkyl thiophene isomer	0.78±0.3
38	147	C_4-alkyl benzene isomer	0.55±0.2
39	149	C_4-alkyl thiophene isomer	0.48±0.2
40	150	C_4-alkyl benzene isomer	1.00±0.2
41	151	$C_{10}H_{12}$ isomer	0.42±0.1
41A	151	C_4-alkyl benzene isomer	T
41B	152	$C_{10}H_{12}$ isomer	T
41C	152	C_4-alkyl benzene isomer	T
41D	153	$C_{10}H_{12}$ isomer	T
42	153	C_5-alkyl benzene isomer	0.38±0.2
42A	154	C_4-alkyl benzene isomer	T

(continued)

Table C27 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
42B	155	C_5-alkyl benzene + methyl benzofuran isomers	40.17±8.0
44	156	C_4-alkyl benzene isomer	0.50±0.2
44A	157	$C_{11}H_{14}$ + C_5-alkyl thiophene isomers	T
45	158	C_5-alkyl benzene isomer	T
46	159	$C_{11}H_{12}$ isomer	1.10±0.5
46A	159	C_5-alkyl benzene + $C_{10}H_{12}$ isomers	T
46B	159	C_5-alkyl benzene isomer	T
47	161	C_5-alkyl benzene isomer	0.48±0.2
48	168	naphthalene	0.71±0.2
48A	169	C_2-alkyl phenol isomer	NQ
48B	171	C_2-alkyl phenol isomer	NQ
48C	179	β-methylnaphthalene	0.08±0

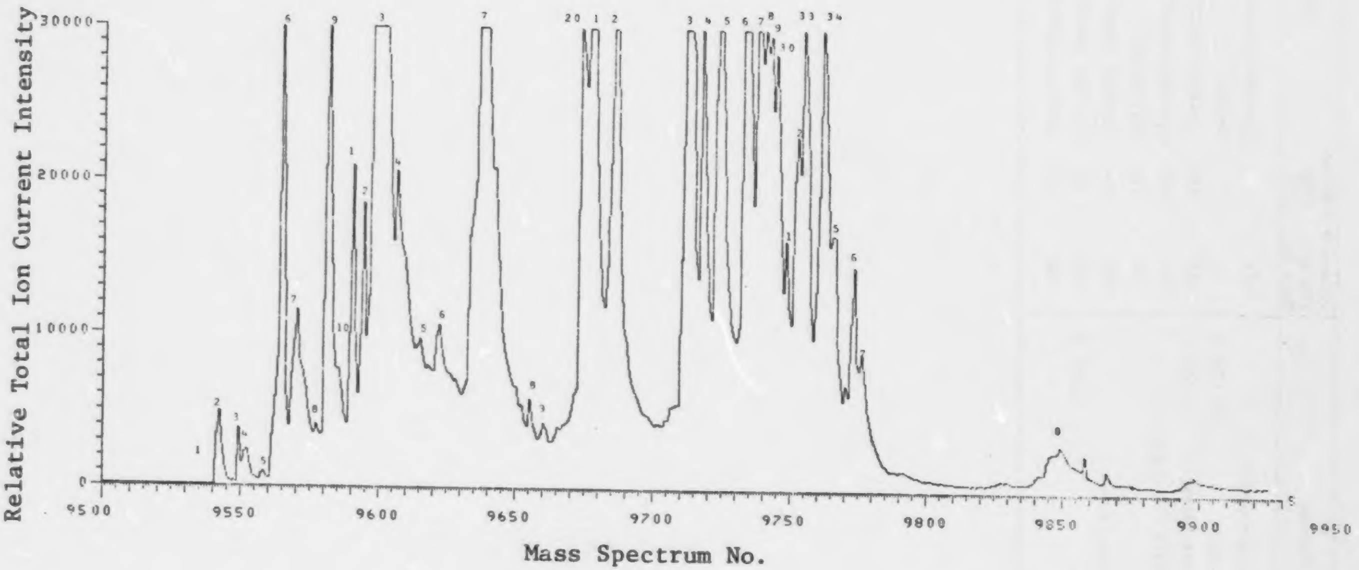


Figure C13. Profile of volatile organics in water sample (-17L) from dewatering well #5, post-gasification (LLL, ERDA).

Table C28. VOLATILE ORGANICS IN WATER (-17L) FROM DEWATERING WELL #5, POST-GASIFICATION (LLL, ERDA)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
2	41	CO_2	–
2A	43	acetaldehyde (tent.)	T
3	45	C_4H_8 isomer	NQ
4	50	C_4H_8 isomer	NQ
4A	52	C_5H_{10} isomer	T
4B	53	C_5H_{12} isomer	T
5A	53	C_5H_{10} isomer	T
6	53	furan	T
6A	53	C_5H_{10} isomer	T
6C	55	carbon disulfide (tent.)	NQ
6D	55	diethyl ether	0.88±0.2
7	56	acetone	5.18±0.4
7A	57	C_5H_8 isomer	T
7B	58	C_5H_{10} isomer	T
8	60	C_6H_{14} isomer	0.59±0.2
9	62	perfluorobenzene (e■)	
9A	62	n-hexane	7.11±0.7
9B	64	C_6H_{12} isomer	9.00±2.1
10	64	C_6H_{10} isomer	T
10A	66	methylcyclopentane	2.86±0.7
11	66	perfluorotoluene (e■)	
12	68	methyl ethyl ketone	2.46±1.0
12A	68	C_6H_{10} isomer	0.37±0.2
13	70	benzene	11.62±1.7
13A	72	thiophene	8.09±1.9
14	74	C_6H_{10} isomer	T
14A	74	methyl isopropyl ketone	2.41±0.6
15	79	C_7H_{12} isomer	T
15A	80	C_7H_{12} isomer	T
15B	81	C_7H_{14} + C_7H_{16} isomers	T
16	82	2-pentanone	2.28±0.7
16A	82	C_7H_{14} isomer	T
16B	83	3-pentanone	9.87±0.4
16C	85	C_7H_{12} isomer	T
17	89	C_2-alkyl furan or C_7H_{12} isomer	T
17A	89	4-methyl-2-pentanone	0.57±0.2
17B	90	2-methyl-3-pentanone	1.27±0.6
17C	91	toluene	58.05±11
17D	91	methylthiophene isomer	17.60±6.0
17E	92	methylthiophene isomer	T
17F	96	3-methyl-2-pentanone	0.50±0.2
17G	98	C_8H_{14} isomer	T
17H	99	C_8H_{18} isomer	T
18A	112	3-hexanone	0.61±0.3
19A	115	$C_6H_{12}O$ isomer	T
19B	119	$C_7H_{14}O$ ketone isomer	T
20	109	ethylbenzene	6.17±1.2
20A	110	C_2-alkyl thiophene isomer	T
21	110	C_2-alkyl thiophene + xylene isomers	52.57±8.0
21A	114	C_2-alkyl thiophene isomer	T
22	115	xylene isomer	53.00±9.5
22A	117	C_2-alkyl thiophene isomer	T
22B	119	C_9H_{18} isomer	T
22C	120	C_9H_{18} isomer	T
22D	121	C_3-alkyl benzene isomer (tent.)	T
22E	125	C_9H_{16} or diethylfuran isomer	T
22F	125	$C_{10}H_{22}$ isomer	T
23	128	C_3-alkyl benzene isomer	2.17±0.2
23A	128	C_3-alkyl thiophene isomer	0.10±0
23B	129	C_3-alkyl benzene isomer	T
23C	129	C_3-alkyl thiophene isomer	T
24	130	C_3-alkyl benzene isomer	0.50±0.1
24A	131	C_3-alkyl thiophene isomer	T
25	132	C_3-alkyl benzene isomer	T
25A	132	benzofuran	28.57±7.0
25B	135	C_3-alkyl thiophene isomer	T
25C	135	$C_{10}H_{20}$ or C_4-alkyl thiophene isomer	T
26	135	C_3-alkyl benzene + C_4-alkyl benzene isomers	T
27	140	indan	23.65±8.9
28	142	indene	61.99±9.9
29	143	C_4-alkyl benzene isomer	0.15±0
29A	144	C_4-alkyl benzene isomer	T
30	145	C_4-alkyl thiophene isomer	1.42±0.4
31	147	C_4-alkyl benzene isomer	T
31A	148	C_4-alkyl thiophene isomer	T
32	149	C_4-alkyl benzene isomer	T
33	150	$C_{10}H_{12}$ isomer	T
33A	152	C_5-alkyl benzene + methylbenzofuran isomer	4.27±0.8
34	153	methylbenzofuran isomer	4.64±1.1
34A	154	C_5-alkyl benzene isomer	T
35	156	C_4-alkyl benzene + C_4-alkyl thiophene isomers	T
35A	156	$C_{10}H_{12}$ + $C_{11}H_{14}$ isomers	T
35B	157	C_6-alkyl benzene isomer	T
36	160	C_5-alkyl benzene isomer	T
36A	160	$C_{10}H_{12}$ isomer	T

(continued)

Table C28 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb	Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
37	162	C_5-alkyl benzene + C_4-alkyl benzene isomers	T			
37A	163	$C_{10}H_{12}$ isomer	T			
37B	164	C_5-alkyl benzene isomer	T			
37C	169	naphthalene	0.22±0.1			
37D	171	C_2-alkyl phenol isomer	NQ			
37E	176	C_2-alkyl phenol isomer	NQ			
37F	186	β-methylnaphthalene	0.16±0.1			
38	196	biphenyl	0.61±0.1			
38A	197	$C_{13}H_{18}$ isomer	T			
38B	199	C_2-alkyl naphthalene isomer	T			

Table C29. VOLATILE ORGANICS IN WATER (-18L) FROM DEWATERING WELL #4, POST-GASIFICATION (LLL, ERDA)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
1	40	CO_2	-
1A	43	2-butene	NQ
2	45	C_5H_{10} isomer	T
2A	46	acetaldehyde	69.80±30
3	47	furan + C_5H_{10} isomer + acetone	58.90±6
3A	47	diethyl ether (tent.)	5.55±1.1
4	48	acetonitrile	1.05±0.2
4A	48	dimethyl sulfide	NQ
5	51	C_5H_8 isomer	T
5A	52	C_5H_{10} isomer	T
6	55	propionitrile	5.28±0.7
7	56	methyl ethyl ketone + hexafluorobenzene (eS)	14.54±6
7A	58	2-thiobutane	0.38±0.1
8	60	methylcyclopentane	0.25±0.1
10	63	perfluorotoluene (eS)	
10A	64	C_6H_{10} isomer	T
11	64	benzene	87.23±9.0
12	67	thiophene + methyl isopropyl ketone	45.36±10
12A	68	3-methyl-2-thiabutane	2.64±0.7
13	69	cyclohexene	0.96±0.3
14	71	2-pentanone	4.76±0.4
15	73	3-pentanone	62.82±8.1
15A	73	C_7H_{12} isomer	T
15B	75	2-thiopentane	T
15C	76	C_7H_{12} isomer	T
15D	77	$C_6H_{12}O$ ketone isomer (tent.)	T
16	81	2,3-dithiabutane	T
17	82	4-methyl-2-pentanone	34.90±8.9
18	83	2-methyl-3-pentanone	51.21±0.2
19	84	toluene + 3-methyl-2-pentanone	87.77±13
20	87	2-methylthiophene	15.71±0.9
21	88	3-methylthiophene	16.81±1.0
22	91	3-hexanone	21.81±5.0
23	92	2-hexanone	41.45±9.9
24	94	thiacyclopentane	0.98±0.2
25	99	cyclopentanone	0.25±0.1
26	101	$C_6H_{10}O_2$ isomer	NQ
27	102	$C_7H_{14}O$ isomer	NQ
28	102	$C_7H_{14}O$ isomer	NQ
29	103	thiacyclohexane	2.18±0.5
29A	103	cyclohexanone	1.81±0.5
30	104	epoxyheptane isomer (tent.)	NQ
31	105	ethylbenzene isomer	44.96±9.9
31A	106	ethylthiophene	3.35±0.9
31B	107	dimethylthiophene isomer	5.00±0.5
32	107	*p* or *m*-xylene	51.37±11
33	109	dimethylthiophene isomer	7.17±0
34	110	hexylnitrile	5.10±1.0
35	111	3-heptanone + dimethylthiophene isomer + styrene	3.77±1.2
36	112	2-heptanone + *o*-xylene	59.55±7.0
37	114	2,4-dimethylthiophene	2.88±0.2
37A	115	$C_8H_{14}O$ isomer (tent.)	T
38	117	anisole	3.44±0.9
39	118	isopropylbenzene + C_3-alkyl thiophene isomer	T
40	119	2,5-dimethylthiacyclopentane	0.52±0.1
40A	120	$C_8H_{16}O$ isomer	T
41	121	methylanisole isomer (tent.)	T
41A	121	$C_8H_{16}O$ isomer	T
42	122	$C_8H_{14}O$ isomer (tent.)	6.75±0.7
43	123	$C_7H_{12}O$ isomer (tent.)	7.77±0.8
44	124	*n*-propylbenzene	T
44A	125	C_3-alkyl thiophene isomer	T
45	126	ethyltoluene isomer	11.42±5.0
46	127	C_3-alkyl thiophene isomer + 1,3,5-trimethylbenzene	3.56±0.9
46A	128	*n*-heptylnitrile	0.78±0.1
47	129	*o*-ethyltoluene	5.41±1.0
47A	129	C_3-alkyl thiophene isomer	T
48	130	3-octanone	3.27±0.5
49	132	2-octanone + 1,2,4-trimethylbenzene	6.42±1.0
49A	133	benzofuran	33.74±1.5
50	136	trimethylthiophene isomer	0.81±0.4
50A	137	methylanisole + C_4-alkyl benzene isomers	0.51±0.1
51	138	1,2,3-trimethylbenzene + C_4-alkyl benzene isomer	125±30
52	140	indan	29.10±5
53	141	indene	1.75±0.9
53A	142	C_4-alkyl benzene isomer	T
54	143	C_4-alkyl benzene isomer	0.55±0.1
54A	144	C_4-alkyl benzene isomer	T
55	144	C_4-alkyl thiophene isomer	1.99±0.9
56	145	C_4-alkyl benzene isomer	2.05±1
57	146	$C_9H_{18}O$ + C_4-alkyl thiophene isomers	2.75±0.4

(continued)

Table C29 (cont'd)

Chromatographic Peak No.	Elution Temp. (°C)	Compound	ppb
57A	146	octylnitrile (tent.) + $C_{10}H_{12}$ isomer	2.35±0.7
58	147	C_4-alkyl benzene isomer	7.98±0.9
59	148	methylindan isomer	1.74±0.6
60	149	C_4-alkyl benzene isomer + 2-nonanone	7.22±2.6
61	151	C_5-alkyl benzene isomer	1.11±0.3
62	152	2-methylbenzofuran	38.11±6.0
63	153	methylbenzofuran isomer	19.00±5.1
64	155	C_4-alkyl benzene isomer	T
65	157	C_5-alkyl benzene isomer	T
65A	157	$C_{11}H_{22}$ isomer	T
66	158	methylindan + C_5-alkyl benzene isomers	
67	160	2,6-dimethylstyrene + $C_{10}H_{10}$ isomer (tent.)	1.51±0.5
67A	160	C_4-alkyl benzene isomer	0.15±0.1
67B	161	C_5-alkyl benzene + methyl indane isomers	0.94±0.1
67C	166	naphthalene	0.22±0.1
67D	169	$C_{10}H_{12}$ isomer	T
68A	215	*n*-pentadecane	0.32±0
68B	220	isopropylnaphthalene isomer	0.08±0
69	222	unknown	
70	223	C_3-alkyl naphthalene isomer + *n*-hexadecane	0.69±0.1

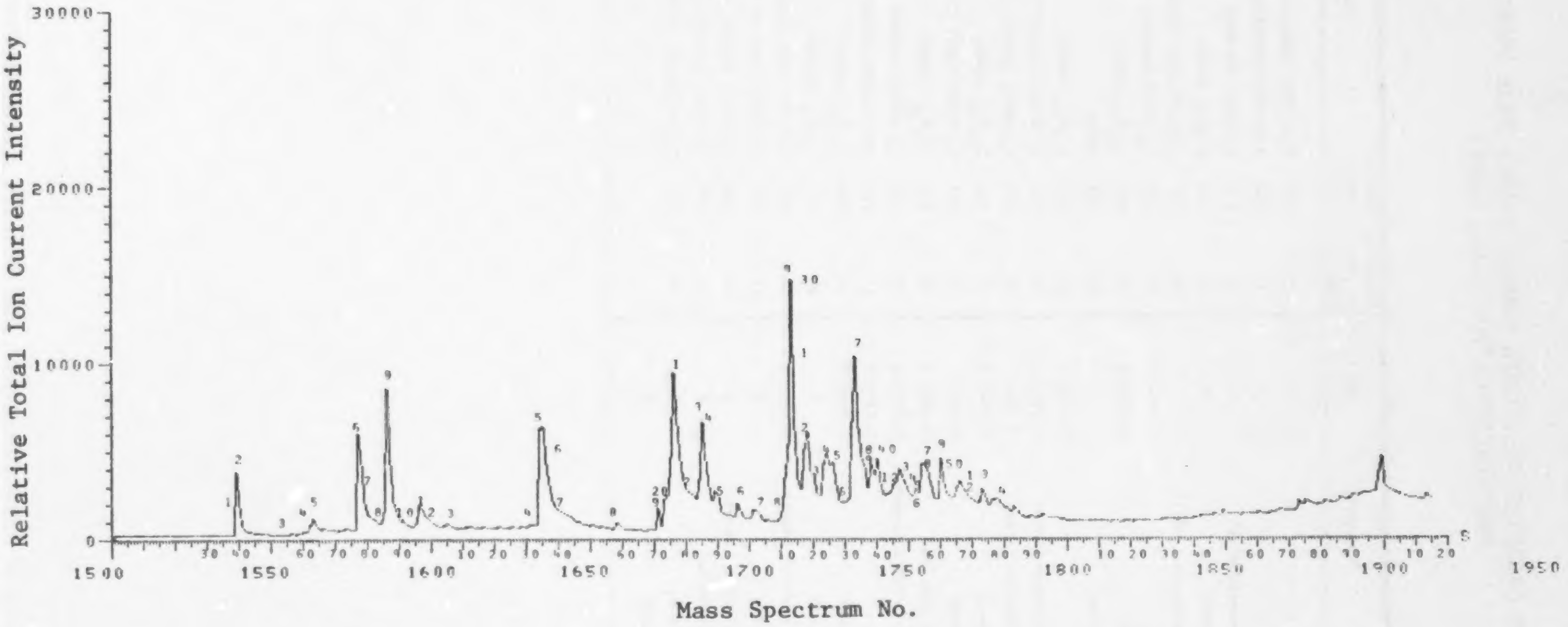


Figure C14. Profile of volatile organics in liquid sample (-19L) from production well #1, post-gasification (LLL, ERDA).

Table C30. VOLATILE ORGANICS IN LIQUID SAMPLE (-19L) FROM PRODUCTION WELL #1, POST-GASIFICATION (LLL, ERDA)

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	ppb
1	40	$N_2 + O_2$	-
2	40	CO_2	-
6	60	perfluorobenzene (eI)	
7	61	C_6H_{14} isomer	T
9	64	perfluorotoluene (eI)	
11	69	benzene	1.07±0.3
12	71	thiophene	0.23±0.1
14	87	C_7H_{12} isomer	T
15	90	toluene	0.58±0.3
16	91	methylthiophene isomer	0.23+0.1
17	92	methylthiophene isomer	0.25±0
19	109	ethylbenzene	0.77±0.4
20	109	C_8H_{16} isomer	0.05±0
21	110	*m*- and/or *p*-xylene	3.08±1.0
22	112	dimethylthiophene isomer	0.19±0.1
23	115	*o*-xylene	1.81±0.4
24	115	C_9H_{18} isomer	0.56±0.2
25	117	C_9H_{20} isomer	T
26	120	C_3-alkyl benzene isomer	0.71±0.3
27	123	C_9H_{18} isomer	T
28	128	C_3-alkyl benzene isomer	T
29	129	C_3-alkyl benzene	T
30	129	C_9H_{18} isomer	T
31	130	C_9H_{18} isomer	T
32	131	C_3-alkyl benzene isomer	0.78±0.3
33	133	trimethylthiophene isomer	0.16±0
34	134	C_3-alkyl benzene isomer	0.61±0.2
35	136	$C_{10}H_{22}$ isomer	0.43±0.2
36	137	C_3H_5-benzene isomer	T
37	139	C_4-alkyl benzene isomer	T
38	140	$C_{10}H_{20}$ isomer	T
39	142	indan	T
40	143	$C_{10}H_{20}$ isomer	T
41	144	C_4-alkyl benzene isomer	T
42	145	C_4-alkyl benzene isomer	T
43	146	$C_{10}H_{20}$ isomer	T
44	148	C_4-alkyl benzene isomer	T
45	149	$C_{10}H_{20}$ isomer	T
46	149	C_4-alkyl benzene isomer	T
47	150	methylindan isomer	T
48	151	$C_{11}H_{22}$ isomer	0.05±0
49	153	$C_{11}H_{24}$ isomer	0.38±0.1
50	156	C_5H_9-benzene isomer	0.10±0
51	157	C_4-alkyl benzene isomer	T
52	158	C_5-alkyl benzene isomer	T
53	160	C_5-alkyl benzene isomer	T
54	162	C_4H_9-benzene isomer	T

Table C31. VOLATILE ORGANICS IN WATER (-20L) FROM PRODUCTION WELL #1, POST-GASIFICATION (LLL, ERDA)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb	Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
1	41	$N_2 + O_2$	-	32	140	C_3-alkyl benzene isomer	T
2	41	CO_2	-	34	156	methylbenzofuran isomer	3.33±1.1
5	45	C_4H_8 isomer	T	35	156	C_3-alkyl benzene isomer	T
7	51	acetaldehyde	T	36	156	C_4-alkyl benzene isomer	T
8	51	furan	0.09±0	37	159	methylindan isomer	T
11	53	propanal	0.67±0.1	38	162	C_4-alkyl benzene isomer	T
12	55	diethyl ether	0.64±0.2	39	167	naphthalene	5.02±1.75
13	56	acetone	1.70±0.5	40	168	C_5H_9-benzene isomer	T
14	58	butyl vinyl ether	T	41	169	dimethylbenzofuran isomer	0.05±0
15	59	perfluorobenzene (eS)		42	172	dimethylbenzofuran isomer	0.03±0
16	60	C_6H_{14} isomer	T	43	172	C_5-alkyl benzene isomer	T
18	64	perfluorotoluene (eS)		44	179	$C_{11}H_{12}$ isomer	0.06±0
20	69	benzene	3.53±1.2	45	181	$C_{12}H_{16}$ isomer	0.07±0
22	89	toluene	6.39±3.0	46	183	C_5-alkyl benzene isomer	T
23	98	C_8H_{18} isomer	T	47	184	methylnaphthalene isomer	T
25	116	C_2-alkyl benzene isomer	0.28±0.1	48	187	$C_{12}H_{16}$ isomer	T
26	120	C_2-alkyl benzene isomer	T	49	196	biphenyl	0.23±0.1
27	121	styrene	0.37±0.1	50	198	$C_{13}H_{18}$ isomer	T
28	129	C_9H_{20} isomer	T	51	200	ethylnaphthalene isomer	0.14±0
29	131	C_3-alkyl benzene isomer	T	52	202	ethylnaphthalene isomer	0.28±0
31	138	benzaldehyde	1.21±0.6				

Table C32. VOLATILE ORGANICS IN PRODUCT TAR (-1L) FROM *IN SITU* COAL GASIFICATION, HANNA #2, PHASE I (LERC, ERDA)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
1	77	SO_2
1A	81	1-butene
1B	82	*n*-butane
1C	83	2-butene
1D	83	C_4H_8 isomer
2	84-9	acetaldehyde
4	92-8	acetone
4A	96	*n*-propyl methyl ether
6	103	cyclopentadiene
6A	104	carbon disulfide
7	104-6	cyclopentene
9	109	*n*-propionitrile
11	111	methyl ethyl ketone
13	119	2-methylpropionitrile
14	123	unknown
15	127	methyl isopropyl ketone + C_6H_{10} isomer
15A	127	benzene
15B	130	thiophene
16	131	2-pentanone
17	133	3-pentanone
18	140	2-methyl-1,5-hexadiene
19	144	*N*-methylpyrrole
19A	145	methyl isobutyl ketone
19B	145	dimethyl sulfide
20	146	pyrrole
21	147	methyl *sec*-butyl ketone
22	149	*n*-butyronitrile
22A	150	toluene
22B	153	methylthiophene isomer
22C	154	3-hexanone
23	155	2-hexanone
24	157	C_7H_{16} isomer
25	159	tetrahydrothiophene + dimethylcyclohexene isomer
26	163	C_8H_{18} isomer
26A	163	2-methylpyrrole
27	165	3-methylcyclopentanone
28	168	thiacyclohexane
29	170	ethylbenzene
30	172	*p*-xylene
30A	174	ethyl butyl ketone
30B	175	2,5-dimethylthiophene + 2-heptanone
31	176	styrene + C_9H_{16} isomer + dimethylthiophene isomer
32	177	*o*-xylene + C_9H_{16} isomer
33	179	2,4-dimethylthiophene
34	180	phenylhydrazine (tent.)
35	183	isopropylbenzene + C_9H_{20} isomer
36	186	*n*-propylbenzene + C_9H_{20} isomer
37	188	*m*-ethyltoluene + trimethylthiophene isomer
38	193	*p*-ethyltoluene + trimethylthiophene isomer
39	196	1,3,5-trimethylbenzene + α-methyl styrene + benzofuran
40	201	*t*-butylbenzene + C_4-alkyl thiophene isomer
41	202	1,2,4-trimethylbenzene
42	205	indan
43	207	indene
44	210	*sec*-butylbenzene
45	212	*o*-cymene
45A	212	*m*-ethylstyrene
46	212	C_4-alkyl benzene isomer
47	214	*n*-undecane + C_4-alkyl benzene isomer
48	216	C_5-alkyl benzene isomer
49	217	2-methylbenzofuran
50	220	C_4-alkyl benzene isomer + 2,6-dimethylstyrene
51	220	C_5-alkyl benzene isomer
52	220	C_5-alkyl benzene isomer
53	220	5-methylindan
53A	220	*n*-pentylbenzene
54	220	3-methylindan
55	220	C_5-alkyl benzene isomer
56	220	1-dodecene
57	220	*n*-dodecane
58	220	naphthalene + 1,3-dimethylindan
58A	220	dimethylbenzofuran isomer
60	220	trimethylindan isomer
61	220	$C_{12}H_{16}$ isomer
62	220	C_6-alkyl benzene isomer
63	220	$C_{13}H_{28}$ isomer
64	220	3-methyl-1,2-dihydronaphthalene
64A	220	$C_{11}H_{14}$ isomer
65	220	1-tridecene

(continued)

Table C32 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
66	220	_n_-tridecane			
67	220	$C_{12}H_{16}$ isomer			
68	220	β-methylnaphthalene			
69	220	α-methylnaphthalene			

Table C33. VOLATILE ORGANICS IN GROUND WATER (-2L) FROM WELL #5 PRIOR TO *IN SITU* COAL GASIFICATION (LERC, ERDA)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
1	42	CO_2	NQ
3	127	toluene	2.5±1
4	145	ethylbenzene	1.7±0.60
5	146	*m*-xylene	0.1±0.10
6	147	*p*-xylene	0.35±0.25
7	150	3-heptanone	0.01±0.01
8	156	styrene	1.2±0.50
9	153	*o*-styrene	0.4±0.01
9A	160	isopropylbenzene	0.02±0.01
10	167	*n*-propylbenzene	0.5±.03
11	170	*m*-ethyltoluene	0.1±.03
11A	170	*p*-ethyltoluene + benzaldehyde	0.10±.03
12	173	1,3,5-trimethylbenzene	0.01±.01
12A	173	$C_{10}H_{20}$ isomer	trace
12B	173	$C_{10}H_{22}$ isomer	0.50±.10
13	175	*o*-ethyltoluene	0.04±.01
14	177	benzofuran	0.05±.01
14A	177	1,2,4-trimethylbenzene	0.03±.02
15	179	$C_{10}H_{20}$ isomer	0.05±.04
16	180	*n*-decare	trace
16A	181	$C_{10}H_{20}$ isomer	trace
17	183	C_4-alkyl benzene isomer	trace
18	184	C_9H_{10} isomer (?)	trace
19	185	1,2,3-trimethylbenzene	0.1±.05
19A	186	C_4-alkyl benzene isomer	0.65±.04
20	190	indene	0.03±.03
20A	190	*p*-propyltoluene	0.10±.05
21	192	*n*-butylbenzene	trace
22	193	$C_{11}H_{24}$ isomer	0.10±.10
23	194	*o*-propyltoluene	0.07±.07
24	195	methylindan	trace
25	196	$C_{11}H_{22}$ isomer	1.4±.85
26	197	ethylheptanal isomer (tent.)	NQ
26A	197	C_4-alkyl benzene isomer	0.01±.01
27	198	methylindan isomer	trace
28	199	*n*-undecane	0.15±.05
29	201	C_5-alkyl benzene isomer	trace
30	202	C_4-alkyl benzene isomer	trace
30A	202	C_5-alkyl benzene isomer	trace
31	203	$C_{12}H_{26}$ isomer	trace
32	204	tetramethylbenzene isomer	0.02±.02
33	205	C_4-alkyl benzene isomer	trace
34	206	dimethylstyrene isomer	0.01±.01
35	207	methylindan isomer	0.03±.03
38	208	C_5-alkyl benzene isomer	trace
38A	209	C_5-alkyl benzene isomer	trace
39	209	$C_{12}H_{24}$ isomer	trace
40	210	$C_{12}H_{24}$ isomer	trace
40A	210	C_5-alkyl benzene isomer	trace
40B	210	methylindene isomer	0.01±.01
41	212	methylindene isomer	trace
42	213	1,2,3,4-tetramethylnaphthalene	0.01±.01
43	215	$C_{12}H_{24}$ isomer	trace
44	216	dimethylindan isomer	0.03±.03
45	218	*n*-dodecane	trace
46	219	naphthalene	2.7±.15
47	220	dimethylindan isomer	0.06±.05
47A	220	dimethylindan isomer	0.08±.03
48	223	C_6-alkyl benzene isomer	trace
49	227	$C_{13}H_{26}$ isomer	trace
50	232	$C_{14}H_{30}$ isomer	0.2±.05
51	233	trimethylindan isomer	trace
52	235	*n*-tridecane	0.3±.05
53	238	β-methylnaphthalene	177±33
54	240	$C_{12}H_{16}$ isomer	trace
55	isothermal	*n*-tetradecane	0.1±.05
56		$C_{14}H_{28}$ isomer	trace
57		biphenyl	trace
58		ethylnaphthalene isomer	trace
59		ethylnaphthalene isomer	trace
60		$C_{15}H_{30}$ isomer	0.05±.05
61		dimethylnaphthalene isomer	trace
62		dimethylnaphthalene isomer	0.20±.20
63		dimethylnaphthalene isomer	0.15±.15
64		dimethylnaphthalene isomer	0.03±.01
65		$C_{16}H_{34}$ isomer	trace
66		$C_{16}H_{34}$ isomer	trace
67		$C_{15}H_{30}$ isomer	trace
68		*n*-pentadecane	NQ

Table C34. VOLATILE ORGANICS IN GROUND WATER SAMPLE (-4L) FROM WELL #6 PRIOR TO IN SITU COAL GASIFICATION (LERC, ERDA)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
1	55	CO_2	
2	84	hexafluorobenzene (e[illegible])	
3	91	perfluorotoluene (e[illegible])	
4	98	benzene	1.2
5	126	toluene	3.0
6	146	ethylbenzene	1.3
7	149	m- and p-xylene	0.7
8	150	3-heptanone	T
9	152	2-heptanone	T
10	152	styrene	1.5
11	153	o-xylene	0.7
12	153	C_8H_{16} isomer	T
13	161	isopropylbenzene	T
14	168	n-propylbenzene	T
15	169	m-ethyltoluene	0.2
16	170	p-ethyltoluene	T
17	170	benzaldehyde	T
18	173	1,3,5-trimethylbenzene	0.1
19	174	cyanobenzene	0.1
20	175	o-ethyltoluene	0.05
21	178	1,2,4-trimethylbenzene	0.3
22	179	$C_{10}H_{20}$ isomer	T
23	180	n-decane	0.15
24	181	$C_{10}H_{20}$ isomer	T
25	183	C_4-alkyl benzene isomer	T
26	185	1,2,3-trimethylbenzene	0.3
27	188	indan	T
28	188	$C_{10}H_{28}$ isomer	T
29	190	indene	T
30	190	p-propyltoluene	0.07
31	191	m-propyltoluene	T
32	192	n-butylbenzene	0.04
33	193	o-propyltoluene	T
34	195	methylindan isomer	T
35	196	C_4-alkyl benzene isomer	0.2
36	197	C_4-alkyl benzene isomer	T
37	198	$C_{10}H_{12}$ isomer	T
38	198	methylindan isomer	T
39	199	n-undecane	0.2
40	220	C_5-alkyl benzene isomer	0.1
41	201	C_5-alkyl benzene isomer	T
42	202	C_4-alkyl benzene isomer	T
43	203	$C_{12}H_{26}$ isomer	T
44	205	methylindan isomer	T
45	209	methylindene isomer	0.2
46	212	methylindene isomer	T
47	213	C_5-alkyl benzene isomer	0.15
48	213	1,2,3,4-tetramethylnaphthalene	0.05
49	215	$C_{12}H_{24}$ isomer	T
50	215	C_6-alkyl benzene isomer	T
51	216	dimethylindan isomer	T
52	217	n-dodecane	0.4
53	218	naphthalene	3.5
54	221	C_6-alkyl benzene isomer	T
55	227	$C_{13}H_{26}$ isomer	T
56	228	$C_{13}H_{28}$ isomer	T
57	235	n-tridecane	0.2
58	238	β-methylnaphthalene	2.0
59	240	C_7-alkyl benzene isomer	T
60	240	$C_{15}H_{32}$ isomer	T
61	240	n-tetradecane	0.3
62	240	ethylnaphthalene	T

Table C35. VOLATILE ORGANICS IN GROUND WATER (-5L) FROM WELL #5 PRIOR TO *IN SITU* COAL GASIFICATION (LERC, ERDA)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
1	128	toluene	2.0±1
3	145	ethylbenzene	1.5±0.5
4	147	*p*-xylene	0.5±.25
4A	150	3-heptanone	trace
5	152	styrene	1.0 ±.5
6	153	*o*-xylene	0.5±.02
6A	161	isopropylbenzene	0.06±.03
8	168	*n*-propylbenzene	0.7±.03
8A	169	*m*-ethyltoluene	0.1±.05
9	170	*p*-ethyltoluene	0.08±.01
10	172	benzaldehyde	trace
10A	173	1,3,5-trimethylbenzene	0.08±.01
10B	173	$C_{10}H_{20}$ isomer	trace
11	174	cyanobenzene	0.06±.01
11B	175	*o*-ethyltoluene	0.08±.02
13	178	1,2,4-trimethylbenzene	0.24±.07
13A	179	$C_{10}H_{20}$ isomer	trace
13B	180	*n*-decane	0.2±.05
13C	181	$C_{10}H_{20}$ isomer	trace
14	183	C_4-alkyl benzene isomer	trace
15	184	C_9H_{10} isomer	trace
16	185	1,2,3-trimethylbenzene	0.3±.04
18	188	$C_{10}H_{20}$ isomer and indan	trace
19	190	indene	trace
19A	190	*p*-propyltoluene	0.08±.01
20	191	*m*-propyltoluene	0.04±.03
20A	192	*n*-butylbenzene	0.04±.03
21	193	$C_{11}H_{24}$ isomer	trace
22	194	*o*-propyltoluene	trace
22A	195	methylindan isomer	trace
23	196	C_4-alkyl benzene isomer	0.2±.04
24	197	C_4-alkyl benzene isomer	trace
24A	198	methylindan isomer	trace
25	199	*n*-undecane	0.2±.03
26	200	C_5-alkyl benzene isomer	0.1±.01
26A	201	C_5-alkyl benzene isomer	0.1±.01
27	202	C_4-alkyl benzene isomer	0.2±.01
27A	202	C_5-alkyl benzene isomer	trace
27B	203	$C_{12}H_{26}$ isomer	trace
28	204	tetramethylbenzene isomer	0.3±.02
29	205	C_4-alkyl benzene isomer	0.2±.01
29A	205	methylindan or dimethylstyrene isomer	trace
30	207	C_5-alkyl benzene isomer	trace
31	208	$C_{12}H_{24}$ isomer and C_5-alkyl benzene isomer	trace
32	210	C_5-alkyl benzene isomer	trace
32A	210	$C_{12}H_{24}$ isomer	trace
32B	211	methylindene isomer	0.04±.01
33	211	C_4-alkyl benzene isomer	NQ
33A	212	C_5-alkyl benzene isomer	NQ
33B	212	methylindene isomer	trace
34	213	C_5-alkyl benzene isomer	NQ
34A	213	1,2,3,4-tetramethylnaphthalene	0.06±.03
35	214	methylindene isomer	trace
35A	215	$C_{12}H_{24}$ isomer	trace
35B	215	C_6-alkyl benzene isomer	trace
36	216	dimethylindan isomer	trace
37	217	*n*-dodecane	0.3±.03
38	218	naphthalene	2.0±.05
39	219	dimethylindan and C_3-alkl indan isomers	trace
40	220	$C_{13}H_{28}$ isomer and C_5-alkyl benzene isomer	trace
41	221	C_6-alkyl benzene isomer	trace
42	222	C_3-alkyl indan isomer	trace
43	223	C_6-alkyl benzene isomer	trace
44	224	C_6-alkyl benzene isomer	trace
44A	224	dimethylindan isomer	trace
45	225	C_6-alkyl benzene isomer	0.2±
46	227	$C_{13}H_{26}$ isomer	trace
47	228	$C_{13}H_{28}$ isomer	trace
48	230	C_6-alkyl benzene isomer	0.4±.05
50	231	$C_{14}H_{30}$ isomer	0.1±.03
51	232	dimethylindan isomer	trace
52	233	trimethylindan isomer	trace
52A	234	$C_{13}H_{26}$ isomer	trace
53	235	*n*-tridecane	0.2±.02
54	237	dimethylindan + trimethylindan isomers	0.1±.05
55	238	β-methylnaphthalene	200
57	240	C_4-alkyl benzene isomer	trace
58	isothermal	$C_{12}H_{16}$ isomer	
59		$C_{12}H_{16}$ and $C_{13}H_{18}$ isomers	trace
60		C_7-alkyl benzene isomer	trace
61		$C_{13}H_{18}$ isomer	trace
62		$C_{15}H_{32}$ isomer	trace
63		$C_{14}H_{28}$ isomer	trace
64		*n*-tetradecane	0.2±.01
65		biphenyl	trace
66	↓	ethylnaphthalene isomer	trace

(continued)

Table C35 (cont'd)

Chromatographic Peak No.	Elution Temp. (°C)	Compound	ppb	Chromatographic Peak No.	Elution Temp. (°C)	Compound	ppb
66A	isothermal	$C_{15}H_{30}$ isomer	0.01±.01				
67		dimethylnaphthalene isomer	0.20±.05				
69		dimethylnaphthalene isomer	0.28±.07				
70		dimethylnaphthalene isomer	0.29±.09				
72		$C_{16}H_{34}$ isomer	0.28±.09				
73		dimethylnaphthalene isomer	0.08±.05				
74		$C_{15}H_{30}$ isomer	trace				
76		n-pentadecane	0.10±.07				

Table C36. VOLATILE ORGANICS IN PRODUCED WATER (-8L) DURING WELL 5-6 *IN SITU* COAL GASIFICATION (LERC, ERDA)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
3	59-61	acetaldehyde	34±5
4	62-6	acetone	9330±100
5	66	acetonitrile	17.0±15
8	72	carbon disulfide	NQ
9	75	*n*-propylamine (tent.)	17.0±2
10	77	C_6H_{10} isomer	NQ
11	79	propionitrile	2000±55
13	83-5	methyl ethyl ketone	5000±0
16	90	2-methylpropionitrile + unknown	100±2
17	92	perfluorotoluene (e[illegible])	-
18A	99	methyl isopropyl ketone	trace
19	99-100	benzene	6670±70
20	101	thiophene	67±18
21	104	*n*-butyronitrile	117±0
22	105	2-pentanone	4700±800
23	107	3-pentanone	2330±500
25	112	α-methylbutyronitrile	17±8
27	115	sulfur compound (?)	NQ
28	116	N-methylpyrrole	33±16
30	118	4-methyl-2-pentanone	67±7
31	120	2-methyl-3-pentanone	83±21
32	122	pyrrole	5000±500
33	123	*n*-pentylnitrile	133±33
34	124	toluene	5000±100
34A	124-132	pyridine	trace
34B	124	2-methylthiophene	trace
35	126	3-methylthiophene + 3-hexanone	330±28
36	127	2-hexanone	670±55
37	129	cyclopentanone	167±35
38	133	C_8H_{18} isomer	33±21
41	140	3-methylpyrrole	1667±170
42	141	2-methylcyclopentanone + 3-methylpyridine	670±225
43	142	2-methylpyrrole	1660±1100
44	144	4-methylpyridine	33±17
45	147	ethylbenzene	1660±10
45A	148	C_8H_{16} isomer	trace
46	149	*p*-xylene	2670±25
47	151	2,5-dimethylthiophene + aniline	67±15 17±8
48	152	2-heptanone	100±50
49	154	styrene	1300±210
49A	154	C_8H_{16} isomer	trace
50	155	*o*-xylene	1300±333
51	157	dimethylpyridine isomer	1670±945
51A	158	C_9H_{20} isomer	trace
52	159	dimethylpyrrole isomer	1000±250
52A	160	dimethylpyridine isomer	trace
52B	161	dimethylpyrrole isomer	trace
53	162	isopropylbenzene + dimethylpyridine isomer	33±17
54	164	ethylpyrrole (tent.)	NQ
55	167	methylpyridine isomer	NQ
56	169	*n*-propylbenzene	167±25
57	170	*m*-ethyltoluene	3300±334
58	171	*p*-ethyltoluene	2.67±1
59	173	2-isopropylthiophene (tent.)	16.7±5
60	174	cyanobenzene	2670±352
60A	174	trimethylpyridine isomer	trace
61	175	*o*-ethyltoluene	2000±299
62	176	$C_{10}H_{20}$ isomer + methylethylpyridine isomer	300±206
63	176	α-methylstyrene	2500±271
63A	177	1,2,4-trimethylbenzene	6670±491
63B	178	benzofuran + *n*-decane	1330±826
63C	179	ethylpyrazine (tent.)	NQ
64	180	trimethylthiophene isomer	1330±279
65	182	C_4-alkyl benzene isomer	167±38
65A	182	$C_{11}H_{24}$ isomer	trace
66	183	1,2,3-trimethylbenzene	2670±811
67	186	dimethylaniline isomer	58±40
67A	187	trimethylpyridine isomer	trace
68	188	indan	1000±210
68A	188-195	phenol	6700±3990
69	190	indene	1000±675
70	191	C_4-alkyl benzene isomer	340±45
71	192	methylcyanobenzene isomer	830±800
72	193	$C_{10}H_{20}$ + C_4-alkyl benzene isomers	23±4
73	195	C_4-alkyl benzene isomer	500±25
74	196	$C_{10}H_{12}$ isomer	840±98
75	197	*o*-cresol	1730±1110
76	198	methylindan isomer	trace
77	199	*n*-undecane	187±91
78	201	methylbenzofuran isomer	3000±117
79	202	2-ethylphenol	1000±177
80	204	C_4-alkyl benzene isomer	670±392
81	205	methylindan isomer + C_5-alkyl benzene isomer	trace trace
81A	206	dimethylindan isomer	trace
82	207	*p*-cresol	1660±778

(continued)

Table C36 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
83	208	C_5-alkyl benzene isomer	0.06±0
84	209	methylindan isomer	00.3±0
84A	210	methylindene isomer	trace
84B	210	$C_{10}H_{12}$ isomer	1.0±1
85	211	C_4-alkyl benzene isomer	1.5±1.5
86	212	m-cresol + C_5-alkyl benzene isomer	2000±670
87	214	3-ethylphenol	5000±1200
	215	$C_{12}H_{24}$ isomer	NQ
88	216	2,4-dimethylphenol	5330±1555
89	218	n-dodecane	4000±100
90	219	naphthalene	13340±134
91	220	dimethylindan isomer + benzothiophene	1340±888
91A	221	C_6-alkyl benzene isomer	trace
92	222	4,7-dimethylbenzofuran	1000±700
93	223	dimethylphenol isomer	trace
94	224	5,6-dimethylbenzofuran	trace
95	225	C_6-alkyl benzene isomer	trace
96	226	C_5-alkyl benzene isomer	trace
97	227	C_6-alkyl benzene + C_3-alkyl phenol isomers	1000±970
98	228	dimethylindene isomer	1660±170
99	229	dimethylindan isomer	1000±170
100	229	1-phenylhexane	67±15
101	230	methyldihydronaphthalene isomer	670±76
102	232	methyldihydronaphthalene + C_3-alkyl indan isomer	800±136
103	233	1-tridecene	900±376
104	235	n-tridecane	5000±500
	236	trimethylindan isomer	NQ
106	237	C_3-alkyl phenol isomer	900±475
107	239	β-methylnaphthalene	2830±284
107A	240	2-isopropylbenzimidazole	trace
108	isothermal	α-methylnaphthalene	2000±100
109		$C_{12}H_{16}$ isomer (tent.)	68±34
110		$C_{13}H_{18}$ isomer	100±52
111		$C_{14}H_{30}$ isomer	117±27
112		C_7-alkyl benzene isomer	150±75
113		$C_{15}H_{32}$ isomer	670±300
114		1-tetradecene	1000±277
		biphenyl	5330±534
115	↓	n-tetradecane	2330±460
116	isothermal	$C_{13}H_{18}$ isomer	trace
117		$C_{13}H_{18}$ isomer	trace
118	↓	ethylnaphthalene isomer	1670±710
118A	240	$C_{12}H_{14}$ isomer	trace
119		dimethylnaphthalene isomer	2000±1120
120		dimethylnaphthalene isomer	670±300
121	↓	dimethylnaphthalene isomer	1330±710
122		$C_{16}H_{34}$ isomer	167±49
123		dimethylnaphthalene isomer	160±130
124		biphenylene + ethylnaphthalene isomer	1700±491
		$C_{15}H_{30}$ isomer	trace
125		n-pentadecane	trace
128		acenaphthene	1690±170
129		isopropylnaphthalene isomer	NQ
130		C_3-alkyl naphthalene isomer	trace
131		tetramethylindan (tent.)	trace
135		trimethylnaphthalene isomer	NQ
137		$C_{16}H_{32}$ isomer	1700±170
138	↓	n-hexadecane	2660±271

Table C37. VOLATILE ORGANICS IN PRODUCED WATER (-9L) FROM WELL 5-6 IN SITU COAL GASIFICATION (LERC, ERDA)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
	43	CO_2	
1	49	1-butene	trace
1A	50	n-butane	trace
1B	58	acetaldehyde	66±3
2	60	dimethyl ether	50±10
3	61-2	acetone	1223±100
3A	63-6	acetonitrile	1340±562
5A	76	n-propylamine	16±7
6	78	propionitrile	2000±120
8	82	methyl ethyl ketone	2340±1000
8A	84	hexafluorobenzene (eI)	-
10	89	isobutyronitrile	83±21
11	91	perfluorotoluene (eI)	-
13	98	benzene and methyl isopropyl ketone	7670±2200
14	100	thiophene	150±50
15	102	n-butyronitrile	1000±110
16	102	2-pentanone	1660±140
17	107	3-pentanone	830±235
19	113	α-methylbutyronitrile	trace
20	115	N-methylpyrrole	25±12
21	117	4-methyl-3-pentanone	34±21
21A	118	$C_6H_{12}O$ isomer	trace
22	120	pyrrole	4000±580
23	121	n-pentylnitrile	1670±295
24	123	toluene	1340±800
24A	124	2-methylthiophene	1000±345
24B	125-6	pyridine and 3-hexanone	trace
24C	128	2-hexanone	330±119
25	132	cyclopentanone	1670±891
27	139	3-methylpyrrole	2330±241
28	140	2-methylcyclopentanone	3000±322
29	141	2-methylpyrrole	2000±775
30	142	methylpyridine isomer	2170±1314
31	144	dimethylpyrrole isomer	1330±610
32	145	n-hexylnitrile	4000±1200
32A	146	ethylbenzene	1330±215
32B	146	C_8H_{16} isomer	330±25
32C	147	methylpyridine isomer	1000±625
33	149	p-xylene	670±111
33A	149	aniline and dimethylthiophene isomer	1330±1100
34	150	3-heptanone	trace
34A	151	dimethylcyclopentanone (tent.)	170±25
35	152	2-heptanone	trace
35A	153	$C_7H_{12}O$ isomer	trace
36	153	styrene	1000±230
36A	154	C_8H_{16} isomer	trace
37	155	o-xylene	1670±717
38	156	cyclohexanone	170±90
39	157	dimethylpyridine isomer	1000±678
40	159	dimethylpyrrole isomer	340±100
40A	160	C_6H_8O isomer (tent.)	trace
40B	161	C_8H_{16} isomer	trace
41	162	dimethylpyridine and methylcyclohexanone (tent.)	340±120
41A	163	C_7H_9N isomer	trace
42	164	dimethylcyclopentanone isomer (tent.)	830±391
43	167	2-methylcyclohexanone	330±29
	169	n-propylbenzene	trace
44	170	benzaldehyde	1340±519
45	171	m-ethyltoluene	350±50
46	172	$C_8H_{14}O$ isomer	trace
47	174	cyanobenzene	1000±117
48	175	o-ethyltoluene	1670±207
49	176	methylpyridine and dimethylpyridine isomers	NQ
49A	177	α-methylstyrene	2000±197
49B	178	1,2,4-trimethylbenzene	1000±25
50	179	benzofuran	trace
51	182	trimethylthiophene isomer	34±9
52	185	1,2,3-trimethylbenzene	3000±198
53	186	phenol	5670±3888
54	188	indan	2340±676
55	190	indene	NQ
56	191	C_4-alkyl benzene isomer	250±28
57	192	methylcyanobenzene isomer	350±32
57A	193	acetophenone	340±120
58	194-6	o-cresol	10000±2000
59	197	C_4-alkyl benzene and methylindan isomers	1230±220
60	198	$C_{10}H_{12}$ isomer	400±111
61	200	methylbenzimidazole (tent.)	300±20
62	201	methylbenzofuran isomer	560±10
62A	202	2-ethylphenol	1000±317
63	204-6	p-cresol	4000±3100
64	209	methylindan isomer	trace
64A	210	methylindene isomer	134±46
65	211	ethylphenol isomer	4200±300
66	212	methylindene isomer	157±39
67	213	dimethylphenol isomer	1330±1075

(continued)

Table C37 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb	Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
68	216	C_3-alkyl phenol isomer	340±110				
68A	217	dimethylphenol isomer	trace				
69	218	dimethylphenol isomer	trace				
70	219	naphthalene	8340±700				
71	220	5,6-dimethylbenzofuran +	34±21				
		dimethylphenol	17±15				
72	222	2-ethylbenzimidazole	50±20				
73	224	dimethylindan	30±20				
73A	224	ethylphenol isomer	trace				
74	225	methylethylphenol isomer	340±100				
75	228	methylethylphenol isomer	350±130				
76	230	dibenzofuran	167±55				
77	232	C_4-alkyl phenol isomer	187±125				
78	233	trimethylphenol isomer	237±100				
79	235	C_4-alkyl phenol isomer	350±217				
80	238	β-methylnaphthalene	1330±121				
82	isothermal	C_3-alkyl phenol	670±477				
83		α-methylnaphthalene	830±56				
84		unknown	NQ				
87		biphenyl					
88		$C_{16}H_{32}$ isomer	trace				
88A		$C_{13}H_{10}$ isomer	trace				
90		ethylnaphthalene isomer	trace				
91		dimethylnaphthalene isomer	67±27				
92		dimethylnaphthalene isomer	67±25				
93		dimethylnaphthalene isomer	116±20				
94		biphenylene	167±92				
95		*n*-pentadecane	83±40				
98		acenaphthene	170±38				
100		diphenylmethane	trace				
102		*n*-hexadecane	trace				

Table C38. VOLATILE ORGANICS IN PRODUCT TAR (-10S) FROM *IN SITU* COAL GASIFICATION (LERC, ERDA)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppm
1	57	acetaldehyde	NQ
2	66	isopentane (tent.)	trace
3	72	acetone	25±10
4	78	dimethylamine (tent.)	NQ
5	85	hexafluorobenzene (e[illegible])	
6	87	*n*-hexane	32±7
7	90	methyl ethyl ketone	75±7
8	92	perfluorotoluene (e[illegible])	
9	100	benzene	1400±1105
10	101	thiophene	76±21
11	102	methyl isopropyl ketone	210±38
12	103	C_7H_{14} isomer	39±23
13	104	2-pentanone	115±72
14	105	*n*-heptane (tent.)	256±121
15	120	α-methylbutyronitrile (tent.)	36±20
16	121	C_8H_{16} isomer	
17	122	4-methyl-2-pentanone	77±31
18	123	2-methyl-3-pentanone	33±11
19	124	3-methyl-2-pentanone	trace
20	125	C_7H_{12} isomer	115±62
21	126	toluene	1132±237
22	127	2-methylthiophene	321±92
23	129	3-methylthiophene	445±85
24	131	3-hexanone	191±46
25	132	C_8H_{16} isomer	62±31
26	133	2-hexanone	299±49
27	134	C_8H_{16} isomer	10±12
28	135	*n*-octane	777±400
29	136	C_8H_{16} isomer	trace
30	137	C_8H_{14} isomer	39±11
31	140	dimethylcyclohexene isomer	75±25
32	142	dimethylheptane isomer	trace
33	144	C_8H_{14} isomer	27±12
34	145	C_8H_{12} isomer	26±10
35	147	C_9H_{18} isomer	22±12
36	149	ethylbenzene	660±230
37	150	propylcyclopentane isomer	48±32
38	150	C_9H_{20} isomer	trace
39	151	*p*-xylene	1910±70
40	152	dimethylthiophene isomer	20±5
41	153	3-heptanone	5±2
42	155	2-heptanone	10±5
43	155	2,3-dimethylthiophene	50±10
44	156	styrene	2200±50
45	156	nonene isomer	440±200
46	157	*o*-xylene	1300±120
47	159	*n*-nonane	1400±150
48	160	C_9H_{18} isomer	220±100
49	160	C_9H_{16} isomer	50±10
50	161	C_9H_{18} isomer	52±11
51	163	C_9H_{18} isomer	trace
52	164	isopropylbenzene	22±12
53	165	dimethylcycloheptane isomer	45±15
54	167	2,6-dimethyloctane	421±100
55	168	C_9H_{18} + $C_{10}H_{20}$ isomer	532±30
56	169	4-*n*-propylheptane	trace
57	170	$C_{10}H_{20}$ isomer	270±105
58	171	*n*-propylbenzene	52±10
59	171	benzaldehyde	40±5
60	172	*m*-ethyltoluene + trimethylcyclohexane isomer	1920±330
61	173	*p*-ethyltoluene	710±340
62	173	1,3,5-trimethylbenzene	110±70
63	174	trimethylcyclohexane + $C_{10}H_{22}$ isomer	˙145±80
64	175	cyanobenzene + C_9H_{10} isomer + octanone isomer	NQ
65	176	*o*-ethyltoluene	2600±200
66	178	$C_{10}H_{20}$ isomer	100±20
67	179	methyl styrene or C_9H_{10} isomer	1600±180
68	180	1,2,4-trimethylbenzene and *n*-decane	1910±190
69	181	C_9H_{20} isomer	50±10
70	182	C_9H_{18} isomer	50±10
71	183	C_9H_{20} isomer	trace
72	183	2,3,4-trimethylthiophene	420±220
73	184	t-butylthiophene or C_4-alkyl thiophene isomer	30±10
74	185	*o*-cymene	35±10
75	185	4-methyldecane	trace
76	186	C_4-alkyl benzene isomer	2100±910
77	186	1,2,3-trimethylbenzene	320±110
78	187	$C_{11}H_{22}$ isomer	
79	188	$C_{11}H_{20}$ isomer	
80	188	C_4-alkyl benzene isomer	1200±710
81	189	indan	3200±1100
82	190	C_4-alkyl benzene + $C_{11}H_{22}$ isomer	120±60
83	191	indene	trace
84	191	C_4-alkyl benzene isomer	1400±100

(continued)

Table C38 (cont'd)

Chromatographic Peak No.	Elution Temp. (°C)	Compound	ppm
85	192	C_4-alkyl benzene isomer	3650±900
86	192	n-butylbenzene	
87	193	C_4-alkyl thiophene isomer	200±50
88	193	$C_{11}H_{24}$ isomer	
89	194	$C_{11}H_{22}$ isomer	42±4
90	195	methylpropylbenzene isomer	15±4
91	196	C_4-alkyl benzene isomer	28±4
92	197	C_4-alkyl benzene + methyl indan isomer	265±35
93	198	undecene	10±2
94	199	methyl indan + C_4-alkyl	990±90
95	200	n-undecane	400±150
96	201	C_5-alkyl benzene isomer	350±100
97	202	2-methylbenzofuran	150±40
98	203	C_5-alkyl benzene isomer	40±10
99	204	C_5-alkyl benzene isomer	10±5
100	204	$C_{12}H_{24}$ isomer	410±220
101	205	C_4-alkyl benzene isomer	250±125
102	206	methylindan isomer	trace
103	206	$C_{11}H_{14}$ isomer	trace
104	208	C_5-alkyl benzene isomer	250±125
105	209	methyl indane or $C_{10}H_{12}$ isomer	175±50
106	210	C_5-alkyl benzene isomer	260±25
107	210	$C_{12}H_{16}$ isomer	300±100
108	211	methyl indene isomer	150±100
109	211	n-pentylbenzene	700±200
110	212	$C_{10}H_{12}$ + C_4-alkyl benzene isomer	300±150
111	213	methyl indene isomer	4200±110
112	214	methylbutylbenzene isomer	1200±100
113	214	1,2,3,4-tetrahydronaphthalene	trace
114	215	C_5-alkyl benzene isomer	2300±800
115	216	dimethyl indan isomer	trace
116	217	cyclododecane (tent.)	trace
117	218-20	n-dodecane and naphthalene	7600±580
118	220	dimethylindan isomer	
119	221	2,6-dimethyl n-decane	420±120
120	222	C_6-alkyl benzene isomer	800±300
121	223	dimethyl benzofuran isomer	400±200
122	224	C_6-alkyl benzene isomer	720±80
123	225	$C_{12}H_{16}$ isomer	50±5
124	226	dimethylbenzofuran + C_6-alkyl benzene isomer	55±25
125	227	$C_{11}H_{14}$ + C_5-alkyl benzene isomer	220±100
126		$C_{13}H_{26}$ isomer	120±50
127	228	$C_{11}H_{12}$ isomer	100±20
128	229	$C_{13}H_{28}$ isomer	140±100
129	230	1-phenylhexane	500±200
130	230	$C_{11}H_{14}$ isomer	200±200
131	231	3,3-dimethylindene	800±250
132	231	7-methyltridecane	910±760
133	232	6-methyl-1,2-dihydronaphthalene	trace
134	233	$C_{12}H_{16}$ isomer	110±20
135	234	1-tridecene	30±10
136	236	n-tridecane	110±60
137	237	$C_{14}H_{28}$ isomer	trace
138	238	$C_{12}H_{16}$ isomer	150±20
139	239	β-methylnaphthalene	4200±1100
140	240	$C_{12}H_{16}$ isomer	220±60
141	isothermal	α-methylnaphthalene	3200±1300
142		$C_{15}H_{32}$ isomer	300±20
143		$C_{14}H_{30}$ isomer	50±25
144		$C_{14}H_{30}$ isomer	trace
145		2,6,10-trimethyldodecane	110±50
146		$C_{14}H_{28}$ isomer	60±10
147		n-tetradecane	1100±500
148		$C_{15}H_{32}$ isomer	trace

Table C39. VOLATILE ORGANICS IN PRODUCT WATER #3 (-11L) DURING WELL 5-6 *IN SITU* COAL GASIFICATION (LERC)

Chromatographic Peak No.	Elution Temp. (°C)	Compound	ppb
4	42	acetaldehyde	NQ
5	43	acetone	NQ
6	44	methyl formate	NQ
7	60-64	*n*-butane	NQ
8	64-67	ethylamine	trace
9	71-73	carbon disulfide	NQ
9A	72-76	cyclopentadiene	
9C	72-76	ethyl nitrate (tent.)	10±5
9D	72-76	C_5H_8 isomer	
10	76-76	nitroethane	
11	77	propane nitrile	445±40
12	80	unknown	NQ
13	81-85	methyl ethyl ketone	600±12
14	86	unknown (m/e 83)	NQ
15	87	C_4H_6 isomer	
16	90	perfluorotoluene (e#)	
17	96-97	methyl isopropyl ketone	50±0
18	97	benzene	600±5
19	98-99	thiophene	620±100
19A	98-100	unknown (m/e 75)	NQ
20	102	methyl *n*-propyl ketone	125±50
21	105	diethyl ketone	40±10
21A	104-107	2-pentanone	100±0
22	111	unknown	NQ
23	112	unknown	NQ
25	116	N-methylpyrrole	1±0
26	117	acetyl acetone	10±5
27	118	pyrrole	210±10
28	119	unknown	NQ
29	121	*n*-pentane nitrile	55±10
30	122	toluene	450±40
30A	~122-124	methylthiophene	55±10
31	125	ethyl *n*-propyl ketone	30±8
32	126	methyl sec-butyl ketone	5±2
34	128	cyclopentanone	30±10
35	132	tetrahydrothiophene	15±5
36	135	pyridine	2420±110
37	137	2-methylpyrrole	24±2
38	140	methyl cyclopentanone	100±15
39	141	methylpyridine isomer	120±1
40	142	C_9H_2O isomer	18±7
43	145	ethylbenzene	220±30
44	146	methylpyridine isomer	trace
45	148	*p*-xylene	500±50
46	150	2,4-dimethylthiophene	50±5
47	151	methylpyridine isomer	trace
48	152	styrene	120±15
49	154	1,4-dimethylbenzene	trace
49A	153-154	aniline or methylpyridine isomer	10±5
50	155	cyclohexanone	trace
50A	155-156	2,3-dimethylthiophene	14±10
51	157	2,5-dimethylpyrrole	7±2
52	158	dimethylpyridine isomer, methylaniline	450±30
53	159-161	M^+/e 105?	NQ
54	161-162	ethylidene cyclopentane	5±4
54A	162	2-pyridone	40±10
55	163-164	$C_7H_{14}O$ isomer	240±100
56	166	C_2-alkyl pyridine or methylaniline	20±10
56A	166	C_3-alkyl furan	5±1
57	168	C_2-alkyl benzene	180±20
58	169	C_3-alkyl benzene	60±7
59	169	2-acetylthiophene (tent.)	38±2
61	172	benzonitrile	40±5
62	173	*o*-ethyltoluene	70±20
64	175-176	aniline	130±20
65	176-177	C_3-alkyl benzene	270±30
66	177	benzofuran	100±20
66A	176-178	methylpyridine isomer	50±20
67	180-181	C_2-alkyl pyridine	trace
67A	180-181	C_3-alkyl thiophene	15±0
67B	180-181	methylacetophenone or dimethylethylbenzene	9±2
68	183	C_3-alkyl benzene	15±5
68A	182-184	*p*-methoxyaniline	
69	185	unknown	
70	186	indane or *o*-methylstyrene	NQ
71	188	indene	340±40
72	191	phenol	265±45
72A	189-192	acetophenone	NQ
73	193-195	*o*-cresol or *m*-cresol	130±35
74	193-196	$C_{11}H_{22}$ isomer	NQ
75	193-196	C_4-alkyl benzene	60±5
76	199	2-methylbenzofuran	20±11
77	200	C_2-alkyl phenol	28±2
78	204	*p*-cresol	NQ
79	206	*n*-butylamine?	NQ
80	208	methylindene	NQ
81	209	C_2-alkyl styrene or methylindane	120±15

(continued)

Table C39 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb	Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
83	211	C_2-alkyl phenol	NQ				
84	214	C_3-alkyl phenol	NQ				
86	217	naphthalene	610±20				
86A	216-217	benzothiophene	110±30				
87	218	C_3-alkyl phenol	NQ				
88	220	C_2-alkyl benzimidazole	trace				
89		C_3-alkyl anisole	trace				
90	237	methylnaphthalene	170±10				
91	238	methylnaphthalene	420±15				

Table C40. VOLATILE ORGANICS IN PRODUCED TAR (-12T) FROM WELL 5-6 *IN SITU* COAL GASIFICATION

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppm
1	59	acetaldehyde (tent.)	trace
2	64	isopentane	trace
3	65	C_5H_{10} isomer	trace
4	67	propanal	trace
5	68	acetone	40±20
6	75	cyclopentene	25±5
6A	79	2-methylpentane	trace
7	83	1-hexene	trace
8	85	hexafluorobenzene (e#)	-
9	86	*n*-hexane	40±10
10	86	3-hexene	42±15
10A	88	methyl ethyl ketone	80±41
10B	91	C_6H_{12} isomer	20±11
11	92	perfluorotoluene (e#)	-
12	95	cyclohexadiene isomer	12±5
12A	98	methylcyclopentene isomer	trace
13	99	benzene	600±76
13A	100	thiophene	60±25
14	103	methyl isopropyl ketone	104±32
15	107	2-pentanone	110±61
15A	108	3-pentanone	44±27
16	110	*n*-heptane	240±100
16A	111	C_7H_{14} isomer	35±21
16B	112	C_7H_{12} isomer	44±11
17	114	C_7H_{12} isomer	50±33
18	118	methylcyclohexane	35±6
19	120	4-methyl-2-pentanone	64±12
20	123	2-methyl-3-pentanone	30±15
21	125	C_7H_{12} isomer	102±51
22	127	toluene	1000±335
22A	128	2-methylthiophene	300±200
23	129	3-methylthiophene	420±171
24	131	3-hexanone	200±127
25	132	2-hexanone	240±120
26	133	C_3-alkyl cyclopentane isomer	trace
26A	134	C_8H_{16} isomer	50±25
27	136	*n*-octane	820±411
28	137	C_8H_{16} isomer	144±100
28A	138	dimethylcyclohexane isomer	80±10
29	141	3-octyne or C_8H_{14} isomer	44±11
30	142	C_9H_{20} isomer	trace
30A	142	1,2-dimethylcyclohexane	32±7
31	143	2-methyloctane	140±47
32	145	C_8H_{14} isomer	34±13
33	146	1-methyl-3-ethylcyclopentane	92±18
33A	147	trimethylcyclohexane isomer	34±17
34	148	1,3,5-trimethylcyclohexane	160±39
34A	149	C_9H_{18} isomer	20±10
34B	149	C_9H_{16} isomer	trace
35	150	ethylbenzene	540±62
36	153	*p*-xylene	1800±67
37	154	2,5-dimethylthiophene	20±10
38	155	C_9H_{18} isomer	51±10
39	157	2,3-dimethylthiophene	48±11
40	158	cyclooctatetraene	1400±49
40A	158	C_9H_{18} isomer	400±100
41	159	*o*-xylene	1200±125
42	160	*n*-nonane	1200±150
43	162	C_9H_{18} isomer	220±110
43A	163	C_9H_{16} isomer	42±7
43B	163	$C_{10}H_{20}$ isomer	20±2
44	164	C_9H_{18} isomer	55±9
45	165	isopropylbenzene	20±10
46	165	$C_{10}H_{18}$ isomer	40±30
46A	166	C_9H_{16} isomer	10±5
47	167	3-methylnonane	360±115
48	169	isopropylcyclohexane and	520±200
		$C_{10}H_{18}$ isomer	trace
49	170	2,3-dimethyloctane	180±85
50	171	$C_{10}H_{20}$ isomer	260±103
51	172	*n*-propylbenzene	40±10
51A	172	$C_{10}H_{20}$ isomer	11±10
52	173	*m*-ethyltoluene and C_9H_{18} isomer	1600±211
53	174	*p*-ethyltoluene	620±349
54	175	2-isopropylthiophene	200±100
55	176	$C_{10}H_{20}$ isomer	140±75
55A	177	$C_{10}H_{18}$ isomer	100±50
56	178	*o*-ethyltoluene	2800±280
57	180	α-methylstyrene and 1-decene	1400±175
58	182	*n*-decane and 1,2,4-trimethylbenzene	1800±175
59	185	2,3,4-trimethylthiophene	400±210
59A	186	*o*-cymene	30±15
60	187	1,2,3-trimethylbenzene	400±110
61	191	indan	3000±1000
61A	191	diethylbenzene isomer	1800±876
62	192	indene and *p*-propyltoluene	1500±170
63	193	*p*-diethylbenzene and *n*-butylbenzene	3800±850
63A	194	ter-butylthiophene isomer	200±55

(continued)

Table C40 (cont'd)

Chromatographic Peak No.	Elution Temp. (°C)	Compound	ppm
64	195	$C_{11}H_{24}$ isomer	2200±200
65	196	*o*-propyltoluene	800±300
65A	196	$C_{11}H_{20}$ + $C_{11}H_{22}$ isomers	40±5
66	197	dimethylethylbenzene isomer	20±2
67	198	dimethylethylbenzene isomer	30±10
68	199	$C_{11}H_{22}$ isomer and 2-methylindane	1100±100
69	201	1-methylindane	1400±410
70	202	*n*-undecane	400±200
71	203	C_5-alkyl benzene isomer	300±100
72	204	methylbenzofuran isomer	156±39
72A	205	C_4-alkyl benzene + C_5-alkyl benzene isomers	50±25
73	206	tetramethylbenzene isomer	1400±230
74	207	C_4-alkyl benzene + $C_{10}H_{12}$ isomer	800±300
74A	208	$C_{11}H_{24}$ isomer	360±210
75	209	C_5-alkyl benzene + C_4-alkyl benzene isomer	400±200
76	210	dimethylstyrene isomer	2200±500
77	211	$C_{12}H_{26}$ + C_5-alkyl benzene isomer	400±200
78	212	*n*-pentylbenzene and $C_{10}H_{12}$ isomer	800±300
79	213	2-methylindene and tetramethylbenzene C_5-alkyl benzene isomers	5800±700
80	214	C_5-alkyl benzene isomer	2400±900
81	216	C_5-alkyl benzene isomer	1800±600
82	217	decanone isomer	80±20
83	219	1-dodecene	200±100
84	220	*n*-dodecane and naphthalene	7400±585
85	221	$C_{11}H_{14}$ isomer	600±100
86	222	$C_{11}H_{14}$ isomer	200±100
87	223	4,7-dimethylbenzofuran	400±300
88	225	C_6-alkyl benzene isomer	800±400
88A	225	$C_{11}H_{14}$ isomer	60±35
89	226	$C_{12}H_{16}$ isomer	50±10
89A	226	C_6-alkyl benzene isomer	60±50
90	227	$C_{13}H_{26}$ isomer	140±55
90A	227	methylindanone isomer (tent.)	200±175
91	228	dimethylindan and C_6-alkyl benzene isomers	trace 600±300
91A	228	C_7-alkyl benzene isomer	1200±600
92	229	C_6-alkyl benzene + C_6-alkyl cyclohexane isomers (tent.)	600±75
92A	229	trimethylindan isomer	140±50
93	230	$C_{13}H_{20}$ isomer	700±157
94	231	1-phenylhexane	200±28
95	232	3,3-dimethylindene or $C_{11}H_{12}$ isomer	800±335
96	233	$C_{14}H_{30}$ isomer	900±700
97	234	$C_{11}H_{12}$ + $C_{11}H_{14}$ isomers	200±100
97A	234	$C_{12}H_{16}$ isomer	112±57
98	235	tridecene isomer	30±15
99	237	*n*-tridecane	114±70
100	238	C_3-alkyl indane isomer	900±350
101	239	$C_{12}H_{16}$ isomer	200±150
102	240	β-methylnaphthalene	3600±1000
103		$C_{13}H_{16}$ isomer	400±95
104	isothermal	α-methylnaphthalene	3000±1100
105		$C_{12}H_{16}$ isomer	200±50
106		$C_{15}H_{32}$ isomer and diisopropylbenzene	400±77
107		$C_{14}H_{30}$ isomer	50±25
108		*n*-heptylbenzene	540±135
109		$C_{15}H_{32}$ isomer	420±100
109A		$C_{12}H_{14}$ isomer	trace
110		*1*-tetradecene	420±120
111		biphenyl and *n*-tetradecane	1000±400
111A		$C_{15}H_{32}$ isomer	trace
112		$C_{15}H_{30}$ isomer	trace
113		2-ethylnaphthalene	300±122
113A		$C_{13}H_{18}$ isomer	68±58
114		dimethylnaphthalene isomer	600±155
114A		1-ethylnaphthalene	560±261
115		dimethylnaphthalene isomer	1400±795
116		dimethylnaphthalene isomer	2200±50
117		$C_{16}H_{34}$ isomer	NQ
118		dimethylnaphthalene isomer	NQ
119		biphenylene	100±50
119A		$C_{15}H_{30}$ isomer	NQ
120		*n*-pentadecane	NQ
121		acenaphthene	NQ
122		isopropylnaphthalene isomer	NQ
123		C_3-alkyl naphthalene isomer	NQ
125		dibenzofuran	NQ
126		C_3-alkyl naphthalene isomer	NQ
127		C_3-alkyl naphthalene isomer	NQ
128		*n*-hexadecane	NQ

Table C41. VOLATILE ORGANICS IN PRODUCED WATER (-13L) FROM WELL 5-6 IN SITU COAL GASIFICATION (LERC, ERDA)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
1	42	CO_2	NQ
2	45	carbonyl sulfide	NQ
2A	48	1-butene	NQ
3	49	n-butane	NQ
6	61-3	acetone	1243±0
7	61-4	acetonitrile	620±60
9	70	carbon disulfide	NQ
11	77	propionitrile	382±47
13	82	methyl ethyl ketone	645±33
15	88	isobutyronitrile	53±16
16	92	perfluorotoluene (eN)	-
16A	96	methyl isopropyl ketone	55±5
17	98	benzene	607±6
18	100	n-butyronitrile	267±13
18A	101	thiophene	620±6
19	104	2-pentanone	124±111
20	106	3-pentanone	55±0
21	112	α-methylbutyronitrile	32±9
22	115	N-methylpyrrole	2±0
23	116	4-methyl-2-pentanone	148±80
24	118	pyrrole	208±21
25	121	n-pentylnitrile	53±0
26	123	toluene + methylthiophene	556±200
		+ pyridine	2222±4
27	124	3-hexanone	27±8
28	125	cyclopentanone	32±9
29	127	n-octane	1±0
31	133	sulfur compound (?)	NQ
32	135	3-methylpyrrole	46±4
33	138	2-methylcyclopentanone	101±10
		+ 2-methylpyrrole	24±2
34	140	methylpyridine isomer	120±11
35	141	C_9H_{20} isomer	17±7
36	143	ethylbenzene	222±27
36A	144	C_8H_{16} isomer	4±0.3
37	146	p-xylene	561±60
38	148	2,4-dimethylthiophene	15±0
39	149	2-heptanone	5±0
40A	151	2,3-dimethylthiophene	52±3
40	152	styrene + C_9H_{18} isomer	118±11
41	153	o-xylene	472±37
42	155	n-nonane +	39±12
		dimethylpyridine isomer	74±15
43	157	dimethylpyridine + C_9H_{18} isomers	417±7
44	158	dimethylpyrrole isomer	7±1
45	160	isopropylbenzene	11±0
	160	$C_{10}H_{20}$ isomer	209±7
46	161	$C_{10}H_{18}$ isomer	5±0
47	163	C_3-alkyl cyclohexane isomer	57±2
48	165	$C_{10}H_{22}$ isomer	27±8
49A	167	$C_{10}H_{20}$ isomer	11±5
49	168	n-propylbenzene	28±3
	169	$C_{10}H_{20}$ + trimethylcyclohexane isomers	96±14
50	170	m-ethyltoluene	184±16
51	170	p-ethyltoluene	61±7
52	171	2-isopropylthiophene	38±16
52A	172	$C_{10}H_{20}$ + $C_{10}H_{22}$ isomers	21±0.3
53	172	trimethylpyridine isomer	40±2
53A	173	cyanobenzene	44±5
54	175	o-ethyltoluene	67±17
56	177	$C_{10}H_{20}$ isomer	30±2
57A	178	α-methylstyrene + $C_{10}H_{20}$	349±42
57	180	1,2,4-trimethylbenzene +	267±27
		n-decane + benzofuran	111±16
58	182	$C_{10}H_{20}$ +	11±0.6
		trimethylthiophene isomers	15±0
58A	184	C_4-alkyl benzene isomer	6±2
59	186	C_4-alkyl benzene isomer	9±3
60	187	C_3-alkyl pyridine isomer	15±3
61	189	indan	334±33
61A	190	phenol	NQ
62	181	indene	272±32
63	192	C_4-alkyl benzene isomer	71±20
63A	193	C_4-alkyl benzene isomer	20±7
64	193	$C_{11}H_{24}$ isomer	57±5
65	195	C_4-alkyl benzene isomer	22±11
66	197	C_4-alkyl benzene isomer + o-cresol	NQ
67	198	$C_{11}H_{22}$ + C_4-alkyl benzene isomers	95±32
68A	201	C_5-alkyl benzene isomer	139±21
69	203	methylbenzofuran isomer	28±4
70	205	p-cresol	NQ
71	206	C_4-alkyl benzene isomer	12±6
71	207	dimethylindan isomer	47±3
72	208	C_5-alkyl benzene isomer	69±13
73A	209	C_5-alkyl benzene isomer	12±1
73	210	methylindan isomer	126±15

(continued)

Table C41 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
73B	211	$C_{12}H_{26}$ + methylindene isomers	184±164
74A	212	C_5-alkyl benzene isomer	12±1
74	212	$C_{10}H_{12}$ + C_4-alkyl benzene isomers	63±15
75	213	methylindene isomer	196±31
76	215	dimethylphenol + C_5-alkyl benzene isomers	NQ
76A	216	C_5-alkyl benzene isomer	T
	217	dimethylindan isomer	T
77	218	1-dodecene	13±5
78	220	*n*-dodecane	86±8
79	221	naphthalene	640±32
79A	222	dimethylindan + C_6-alkyl	162±15
		benzene isomers	42±5
		benzothiophene	118±6
80	224	dimethylbenzofuran isomer	148±22
81	225	$C_{12}H_{16}$ + C_6-alkyl benzene isomers	56±4
82	227	$C_{11}H_{14}$ isomer	11±0
83	228	dimethylindene + C_6-alkyl benzene isomers	17±7
	229	trimethylindan isomer	22±0
84	230	$C_{13}H_{28}$ isomer	NQ
85	231	$C_{11}H_{14}$ + C_6-alkyl benzene isomers	NQ
86	232	dimethylindene + $C_{14}H_{30}$ isomers	50±10
87	233	dimethylindan + dimethylindene isomers	128±11
88	235	1-tridecene + trimethyl-	12±0.7
		indan isomer	94±7
89	237	*n*-tridecane	222±11
90	238	trimethylindan isomer	111±15
92	240	α-methylnaphthalene	162±16
93	isothermal	β-methylnaphthalene	345±7
94		2-isopropylbenzimidazole (tent.)	25±2
95		$C_{13}H_{18}$ isomer	11±0
96		$C_{14}H_{30}$ isomer	19±4
97		*n*-heptylbenzene	26±5
98		$C_{15}H_{32}$ isomer	21±6
99		1-tetradecene	47±4
99A		biphenyl	114±12
100		*n*-tetradecane	129±14
101		$C_{13}H_{18}$ isomer	16±7
102		ethylnaphthalene isomer	39±9
103		dimethylnaphthalene isomer	195±17
104		dimethylnaphthalene isomer	100±12
105		dimethylnaphthalene isomer	135±52
106		$C_{16}H_{23}$ isomer	26±11
107	isothermal	dimethylnaphthalene isomer	47±14
108		ethylnaphthalene isomer	69±21
109		*n*-pentadecane	T
111		acenaphthene	612±9
112		isopropylnaphthalene isomer	
113		$C_{18}H_{28}$ isomer (tent.)	T
114		$C_{14}H_{20}$ isomer	31±5
115		trimethylnaphthalene isomer	7±1
117		C_3-alkyl naphthalene isomer	5±1
119		C_3-alkyl naphthalene isomer	7±0
119A		methyl acenaphthene isomer	15±3
120		C_3-alkyl naphthalene isomer	T

Reproduced from best available copy.

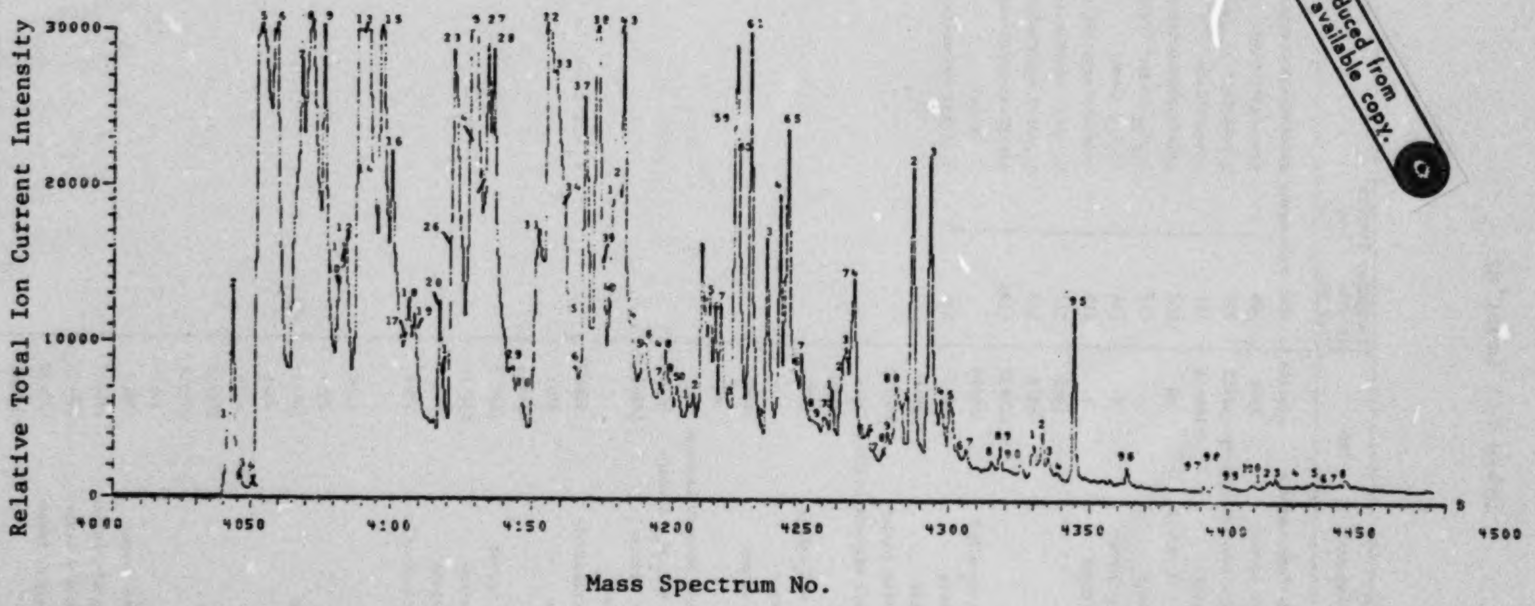


Figure C15. Profile of volatile organics in product water sample (-14L) in situ coal gasification (LERC, ERDA).

Table C42. VOLATILE ORGANICS IN PRODUCED WATER (-14L) FROM WELL 7-8 *IN SITU* COAL GASIFICATION (LERC, ERDA)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
1	41	CO_2	-
3	43	1-butene	0.73±0
4	46	acetaldehyde	NQ
5	47	acetone + ethane nitrile	6456±5800
6	50	CS_2	NQ
6A	51	C_3H_9N isomer (tent.)	NQ
6B	52	*t*-butanol	
7	53	propane nitrile	1482±100
8	56	methyl ethyl ketone	5578±2400
8A	47	hexafluorobenzene (eS)	
8B	58	C_5H_8 isomer + isobutyronitrile	127±58
11	61	perfluorotoluene (eS)	
13	64	benzene + 3-methyl-2-butanone	3259±125
13A	66	thiophene	118±1
14	67	*n*-butyronitrile (tent.)	242±39
15	68	2-pentanone	927±9
16	71	3-pentanone	525±215
17	73	$C_6H_{12}O$ isomer	31±15
18	73	α-methylbutyronitrile	98±67
19	74	$C_6H_{12}O$ isomer	25±5
19A	77	*N* methylpyrrole	17±3
20	79	4-methyl-2-pentanone	27±0
22	80	2-methyl-3-pentanone	235±76
23	81	pyrrole	446±121
24	84	*n*-pentane nitrile	110±0
25	85	toluene	235±59
25A	86	2-methylthiophene	65±0
26	87	3-methylthiophene	72±21
27	88	3-hexanone + cyclopentanone	185±28
28	89	2-hexanone	51±5
28A	90	sulfur compound	NQ
29	91	methylcyclopentanone	100±38
30	93	*n*-octane	7±0.6
31	96	2-methylpyridine	143±100
32	98	3-methylpyrrole + 2-methyl-cyclopentanone	109±64
33	99	2-methylpyrrole	NQ
34	101	$C_7H_{14}O$ isomer	16±24
35	101	methylpyridine isomer	37±7
36	102	4-heptanone ($C_7H_{14}O$ isomer)	T
36A	103	dimethylpyrrole isomer	17±1
37	104	ethylbenzene	742±8
37A	105	dimethylthiophene isomer	T
38	106	*p*-xylene	232±1
39	107	dimethylthiophene isomer	71±33
40	108	3-heptanone	9±3
41	109	2-heptanone + $C_7H_{12}O$ isomer	151±62
42	109	styrene + dimethylpyridine isomer	162±22
43	110	*o*-xylene	224±7
44	112	dimethylpyridine + dimethyl-thiophene isomers	132±50
45	114	dimethylpyrrole isomer	T
46	115	ethylpyridine isomer	38±30
47	117	isopropylbenzene	6±5
48	118	$C_8H_{14}O$ isomer	T
49	119	1-ethylpyrrole	31±0
50	120	2-methylcyclohexanone	5±3
51	122	benzaldehyde	2±1
51A	123	*n*-propylbenzene	T
52	123	C_7H_9N isomer	10±3
52A	124	$C_8H_{14}O$ isomer	NQ
53	125	*m*-ethyltoluene	370±33
54	125	C_3-alkylpyridine isomer	NQ
55	126	cyanobenzene	39±4
56	127	$C_{10}H_{22}$ isomer	197±39
57	128	*o*-ethyltoluene	29±3
58	129	2-octanone	T
59	131	benzofuran	164±41
60	132	1,2,4-trimethylbenzene	T
63	136	1,2,3-trimethylbenzene	137±55
63A	137	C_4-alkyl benzene isomer	64±33
64	139	indan	456±45
65	140	indene	2215±239
66	142	propyltoluene isomer	5±3
67	143	acetophenone	10±3
68	144	$C_9H_{16}O$ isomer	NQ
68A	145	C_4-alkyl benzene isomer	6±2
69	146	$C_{11}H_{24}$ isomer	T
69A	147	C_4-alkyl benzene isomer	T
70	147	C_4-alkyl benzene + methylindan isomers	87±35
71	148	dimethylstyrene or methylindan isomers	5±1
71A	149	C_4-alkyl benzene isomer	T
71B	150	vinylbenzaldehyde or methyl-benzofuran isomer	40±37
72	150	dimethylphenol isomer	NQ
73	151	2-methylbenzofuran	28±3
74	152	*n*-undecane	93±13
75	154	*n*-butylbenzene	21±9
76	155	*m*-propyltoluene	9±7

(continued)

Table C42 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb	Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
77	156	C_4-alkyl benzene isomer					
77A	157	C_5-alkyl benzene isomer	T				
78	158	methylindan isomer					
79	158	C_5-alkyl benzene isomer	T				
79A	159	methylindene isomer	T				
80	160	methylindan isomer	T				
80A	160	C_4-alkyl benzene isomer	T				
81	161	methylindene + C_5-alkyl benzene isomers	20±9				
81A	161	n-pentylbenzene	10±7				
82A	164	C_5-alkyl benzene isomer	33±9				
83	166	naphthalene	154±17				
84	168	dimethylindan isomer	31±17				
85	169	n-dodecane	96±12				
86	171	4,7-dimethylbenzofuran	T				
87	172	$C_{13}H_{28}$ isomer	T				
88	177	dimethylindan isomer	3±0.7				
89	178	C_5-alkyl benzene isomer					
90	182	C_6-alkyl benzene + $C_{14}H_{30}$ isomers					
91	184	β-methylnaphthalene	28±11				
92	186	n-tridecane	42±10				
93	187	α-methylnaphthalene	8±4				
94	188	C_3-alkyl indan isomer	4±3				
95A	198	$C_{14}H_{30}$ isomer	T				
96	201	n-tetradecane	25±3				
97	215	n-pentadecane	T				
103	229	n-hexadecane	NQ				
108	240	n-heptadecane	NQ				

Table C43. VOLATILE ORGANICS IN PRODUCED TAR (-15T) FROM WELL 7-8 *IN SITU* COAL GASIFICATION (LERC, ERDA)

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	ppm	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	ppm
3	40	O_2	-	57	101	C_9H_{18} isomer	T
4	40	CO_2	-	58	102	C_9H_{16} isomer	T
6	43	C_4H_8 isomer	NQ	59	104	ethylbenzene	267 ± 26
7	43	C_4H_{10} isomer	NQ	60	104	C_9H_{18} isomer	T
10	48	C_5H_{12} isomer	15 ± 5	61	106	C_9H_{16} isomer	30 ± 15
11	49	acetone	284 ± 212	62	106	C_9H_{20} isomer	162 ± 60
13	53	C_5H_{10} isomer	T	63	107	*p*- or *m*-xylene	4848 ± 500
14	57	perfluorobenzene (eS)		64	107	C_9H_{16} isomer	3000 ± 600
15	57	C_6H_{14} isomer	50 ± 20	65	107	C_9H_{18} isomer	
17	60	perfluorotoluene (eS)		66	108	C_9H_{20} isomer	
19	64	benzene	2327 ± 1600	67	110	C_8H_{16} isomer	42 ± 10
20	64	cyclohexane	4.6 ± 0	68	110	C_9H_{18} isomer	10 ± 4
21	64	thiophene	27 ± 3	69	110	styrene	177 ± 18
22	68	C_7H_{16} isomer	T	70	111	*o*-xylene	282 ± 202
23	71	C_7H_{14} isomer	9 ± 3	71	112	C_9H_{16} isomer	2100 ± 440
25	73	C_7H_{12} isomer	T	72	112	C_9H_{18} isomer	
26	73	C_7H_{16} isomer	T	73	113	C_9H_{18} isomer	
27	74	C_7H_{14} isomer	31 ± 13	74	114	C_9H_{20} isomer	30 ± 15
28	76	C_7H_{12} isomer	2 ± 1	75	114	C_9H_{18} isomer	800 ± 300
29	76	C_7H_{14} isomer	T	76	114	C_9H_{16} isomer	
30	77	diisopropanolamine (tent.)	NQ	77	116	C_9H_{18} isomer	
31	77	C_7H_{14} isomer	T	78	116	$C_{10}H_{20}$ isomer	13 ± 3
32	78	C_7H_{16} isomer	5 ± 1	79	117	C_3-alkyl benzene isomer	14 ± 6
33	78	C_8H_{14} isomer	T	80	118	$C_{10}H_{18}$ isomer	T
34	79	C_7H_{14} isomer	6 ± 3.2	81	118	$C_{10}H_{22}$ isomer	T
35	80	C_7H_{12} isomer	T	82	120	C_3-alkyl benzene isomer	3 ± 1.6
36	80	C_7H_{16} isomer	T	83	120	C_9H_{16} isomer	3.4 ± 2.2
37	82	C_8H_{14} isomer	T	84	120	C_9H_{18} isomer	T
38	82	C_7H_{16} isomer	7.4 ± 3.4	85	121	$C_{10}H_{18}$ isomer	40 ± 10
39	82	C_7H_{12} isomer	T	86	121	$C_{10}H_{20}$ isomer	
40	84	toluene isomer	2021 ± 660	87	121	$C_{10}H_{22}$ isomer	
41	86	methylthiophene isomer	46 ± 6	88	122	$C_{10}H_{22}$ isomer	190 ± 80
42	87	C_8H_{18} isomer	23 ± 10	89	122	$C_{10}H_{18}$ isomer	
43	89	C_8H_{16} isomer	3 ± 1.2	90	122	$C_{10}H_{20}$ isomer	
44	89	C_8H_{14} isomer	T	91	123	$C_{10}H_{22}$ isomer	60 ± 30
45	90	C_8H_{16} isomer	15 ± 5	92	125	C_3-alkyl benzene isomer	NQ
46	91	C_8H_{14} isomer	T	93	125	$C_{10}H_{20}$ isomer	22 ± 10
47	92	C_8H_{18} isomer	8 ± 4	94	125	C_9H_{18} isomer	24 ± 12
48	93	C_8H_{14} isomer	90 ± 22	95	125	C_3-alkyl benzene isomer	1200 ± 240
49	93	C_8H_{16} isomer	11 ± 2	96	127	$C_{10}H_{20}$ isomer	T
50	94	C_8H_{14} isomer	4 ± 1	97	128	$C_{10}H_{22}$ isomer	1000 ± 440
51	95	C_8H_{16} isomer	T	98	128	$C_{10}H_{20}$ isomer	120 ± 43
52	96	C_8H_{14} isomer	T	99	128	C_3-alkyl benzene isomer	42 ± 12
54	99	C_9H_{20} isomer	15.2 ± 6	101	129	$C_{10}H_{18}$ isomer	10 ± 5
55	100	C_8H_{16} isomer	17 ± 8	102	130	$C_{10}H_{20}$ isomer	T
56	100	C_8H_{14} isomer	6 ± 2	103	132	methylstyrene isomer	T

(continued)

Table C43 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppm
104	132	$C_{10}H_{20}$ isomer	1300 ± 240
105	133	$C_{10}H_{18}$ isomer	
106	133	$C_{10}H_{20}$ isomer	1380 ± 260
107	133	$C_{10}H_{22}$ isomer	
109	134	$C_{10}H_{22}$ isomer	
110	134	$C_{10}H_{20}$ isomer	420 ± 200
111	134	C_4-alkyl benzene isomer	624 ± 170
112	134	$C_{10}H_{18}$ isomer	T
113	134	$C_{11}H_{22}$ isomer	T
114	135	$C_{10}H_{20}$ isomer	1130 ± 400
115	136	C_4-alkyl benzene isomer	
116	138	$C_{10}H_{20}$ isomer	
117	139	$C_{11}H_{24}$ isomer	1100 ± 300
118	139	methylstyrene isomer	
119	140	$C_{11}H_{22}$ isomer	
120	141	methylphenylacetylene	119 ± 118
121	142	C_4-alkyl benzene isomer	380 ± 280
122	143	$C_{11}H_{22}$ isomer	500 ± 200
123	143	$C_{11}H_{20}$ isomer	
124	144	$C_{11}H_{22}$ isomer	
125	144	C_4-alkyl thiophene isomer	12 ± 6
126	145	$C_{11}H_{24}$ isomer	40 ± 15
127	146	C_4-alkyl benzene isomer	
128	146	$C_{11}H_{20}$ isomer	
129	147	$C_{11}H_{24}$ isomer	40 ± 15
130	147	dimethylstyrene isomer	T
131	147	$C_{11}H_{22}$ isomer	22 ± 5
132	148	C_4-alkyl benzene isomer	21 ± 6
133	148	dimethylstyrene isomer	T
134	148	$C_{11}H_{20}$ isomer	53 ± 20
135	148	C_4-alkyl benzene	T
136	149	C_4H_7-benzene isomer	T
137	150	$C_{11}H_{20}$ isomer	1700 ± 300
138	151	$C_{11}H_{22}$ isomer	
139	152	$C_{12}H_{24}$ isomer	
140	152	methylbenzofuran isomer	115 ± 12
141	152	C_5-alkyl benzene isomer	920 ± 300
142	152	$C_{11}H_{22}$ isomer	
143	153	$C_{11}H_{24}$ isomer	
144	153	$C_{11}H_{22}$ isomer	
145	155	C_5-alkyl benzene isomer	25 ± [illegible]
146	155	C_4-alkyl benzene isomer	T
147	156	$C_{12}H_{26}$ isomer	14 ± 4
148	156	$C_{12}H_{18}$ isomer	
149	156	$C_{12}H_{20}$ isomer	
150	156	$C_{12}H_{22}$ isomer	
151	156	$C_{12}H_{24}$ isomer	T
152	156	C_5-alkyl benzene isomer	T
153	156	C_5-alkyl benzene isomer	T
154	158	C_5-alkyl benzene isomer	62 ±
155	159	C_4-alkyl benzene isomer	620 ± 280
156	159	C_5-alkyl benzene isomer	
157	160	$C_{11}H_{22}$ isomer	
158	160	C_5-alkyl benzene isomer	
159	160	methylindene isomer	137 ± 14
160	161	C_4-alkyl benzene isomer	T
161	161	$C_{11}H_{22}$ isomer	10 ± 2
162	161	C_5-alkyl benzene isomer	T
163	162	*n*-pentylbenzene	52 ± 51
164	162	C_5-alkyl benzene isomer	T
165	163	C_5-alkyl benzene isomer	30 ± 5
166	163	$C_{12}H_{22}$ isomer	
167	163	$C_{12}H_{24}$ isomer	
168	163	$C_{12}H_{26}$ isomer	
169	164	C_5-alkyl benzene isomer	
170	164	$C_{12}H_{24}$ isomer	
171	165	$C_{12}H_{26}$ isomer	T
172	166	C_5-alkyl benzene isomer	1520 ± 260
173	166	C_5-alkyl benzene isomer	
174	168	$C_{12}H_{26}$ isomer	
175	168	naphthalene	918 ± 222
176	168	C_5-alkyl benzene	NQ
177	168	$C_{12}H_{24}$ isomer	NQ
178	168	C_6-alkyl benzene isomer	NQ
179	168	dimethylindan isomer	50 ± 3.2
181	171	dimethylindene isomer	56 ± 11
182	171	dimethylbenzofuran isomer	114 ± 5
183	171	$C_{12}H_{26}$ isomer	40 ± 11
184	171	$C_{12}H_{24}$ isomer	
185	171	C_6-alkyl benzene isomer	30 ± 12
186	172	$C_{13}H_{26}$ isomer	15 ± 5
188	172	trimethylindan isomer	11 ± 4
189	172	$C_{12}H_{24}$ isomer	30 ± 10
190	173	$C_{13}H_{28}$ isomer	
191	173	$C_{13}H_{26}$ isomer	
192	173	C_6-alkyl benzene isomer	T
193	174	C_2-alkyl dihydroindene isomer	5 ± 2
194	175	$C_{12}H_{26}$ isomer	T
195	175	$C_{13}H_{26}$ isomer	T
196	175	C_6-alkyl benzene isomer	4 ± 2
197	176	C_6-alkyl benzene isomer	3 ± 1
198	176	C_6-alkyl benzene isomer	11 ± 1

(continued)

Table C43 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppm	Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppm
199	176	$C_{13}H_{26}$ isomer					
200	176	$C_{12}H_{22}$ isomer	T				
201	178	C_6H_{11}-benzene isomer	NQ				
202	179	C_7-alkyl benzene isomer					
203	179	$C_{13}H_{26}$ isomer	T				
204	180	dimethyldihydroindene isomer	T				
205	181	C_6-alkyl benzene isomer					
206	182	$C_{11}H_{14}$ isomer	T				
207	183	$C_{13}H_{28}$ isomer					
208	184	$C_{14}H_{30}$ isomer					
209	185	β-methylnaphthalene					
210	185	$C_{14}H_{28}$ isomer					
211	186	$C_{13}H_{28}$ isomer	T				
212	187	$C_{13}H_{26}$ isomer	T				
213	187	C_6H_{11}-benzene isomer	T				
214	187	$C_{14}H_{28}$ isomer	T				
215	188	α-methylnaphthalene					
216	189	C_7-alkyl benzene isomer	T				
217	192	$C_{14}H_{26}$ isomer	T				
218	192	$C_{14}H_{28}$ isomer	T				
219	193	$C_{13}H_{26}$ isomer	T				
220	194	$C_{14}H_{26}$ isomer					
221	196	phenylpyridine (tent.)					
222	198	$C_{15}H_{32}$ isomer					
223	199	$C_{14}H_{28}$ isomer	T				
224	201	$C_{14}H_{30}$ isomer	T				
225	203	C_2-alkyl naphthalene isomer					
226	206	C_2-alkyl naphthalene isomer					
227	210	biphenylene	T				
228	212	C_2-alkyl naphthalene isomer	T				
229	217	$C_{12}H_{24}$ isomer	T				
230	222	$C_{12}H_{26}$ isomer	T				
231	223	$C_{12}H_{24}$ isomer	T				
232	224	dibenzofuran					
233	224	$C_{12}H_{26}$ isomer	T				
234	225	1,3-dihydro-4,6-dimethyl-thienothiophene (tent.)					
235	227	C_3-alkyl naphthalene isomer	T				
236	228	$C_{13}H_{28}$ isomer	T				
237	231	C_3-alkyl naphthalene isomer	T				
238	235	$C_{13}H_{28}$ isomer	T				
239	238	$C_{13}H_{26}$ isomer	T				
240	240	$C_{16}H_{34}$ isomer	T				
241	240	$C_{14}H_{30}$ isomer	T				

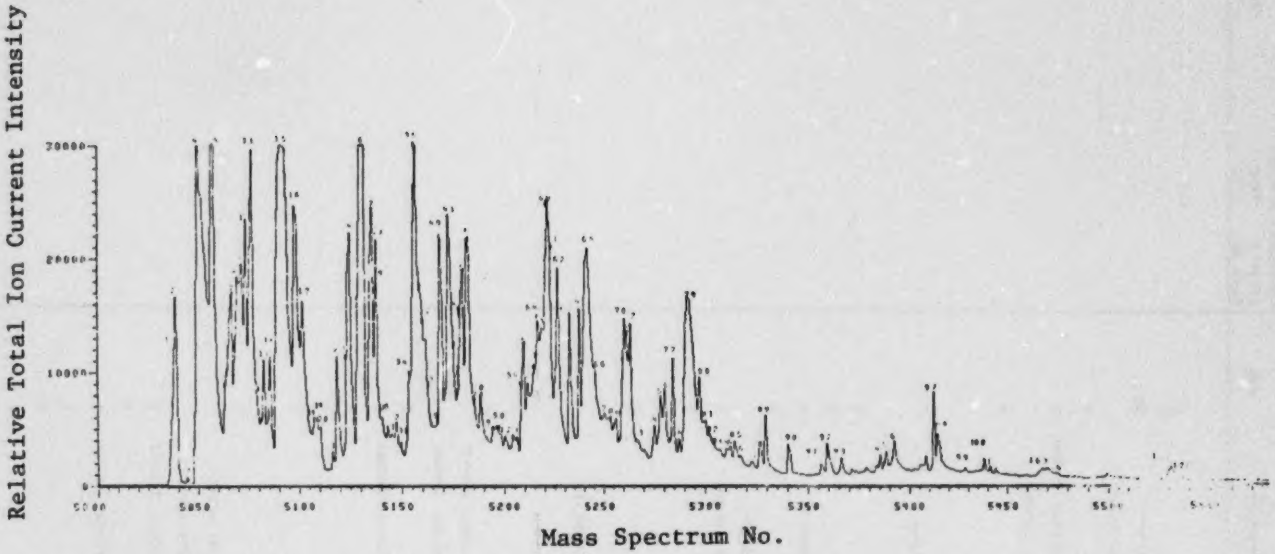


Figure C16. Profile of volatile organics in product water sample (-16L) during well 7-8 in situ coal gasification (LERC, ERDA).

Table C44. VOLATILE ORGANICS IN PRODUCED WATER (-16L) FROM WELL 7-8 IN SITU COAL GASIFICATION (LERC, ERDA)

Chromatographic Peak No.	Elution Temp. (°C)	Compound	ppb
1	40	CO_2	NQ
2A	44	1-butene + n-butane	T
3	45	acetaldehyde	2033 ± 835
4	48	acetone	2545 ± 1299
4A	49	dimethyl ether + diethyl ether	11 ± 12
4B	49	acetonitrile + isopropanol	367 ± 243
4C	50	dimethyl sulfide	668 ± 470
5A	52	ter-butanol (tent.)	66 ± 17
7	56	propionitrile	139 ± 70
8	57	C_6H_{14} isomer	T
9	58	methyl ethyl ketone	1391 ± 434
10	59	hexafluorobenzene (e#)	
12	63	methylcyclopentane (tent.)	T
13	64	perfluorotoluene (e#)	
15	68	benzene + methyl isopropyl ketone	2939 ± 798
15B	70	thiophene	228 ± 109
16	71	2-pentanone + n-butyronitrile	753 ± 306
17	73	3-pentanone	284 ± 21
18	76	$C_6H_{12}O$ isomer	T
19	76	α-methylbutyronitrile	167 ± 72
20	77	$C_6H_{12}O$ isomer	T
21	80	N-methylpyrrole	8 ± 5
22	82	4-methyl-2-pentanone	28 ± 9
22A	83	dimethyl disulfide	T
23	84	2-methyl-3-pentanone	45 ± 37
24	85	pyrrole	6661 ± 237
24A	85	3-methyl-2-pentanone	12 ± 3
25	86	n-pentylnitrile	424 ± 209
26	88	toluene	563 ± 171
26A	89	2-methylthiophene	170 ± 37
27	90	3-methylthiophene	193 ± 40
28	90	cyclopentanone + 3-hexanone	141 ± 42
29	91	2-hexanone	64 ± 30
30	92	pyridine	106 ± 70
31	94	thiacyclopentane	29 ± 4
31A	94	sulfur compound	NQ
32	96	n-octane	7.6 ± 1
33	97	vinylthiophene isomer	T
33A	98	acetoxybutene isomer (tent.)	NQ
34	99	2-methylpyridine	72 ± 39
34A	100	2-methylcyclopentanone	73 ± 24
35A	101	cyclohexanone	65 ± 11
36	102	2-methylpyrrole	124 ± 4
37	103	5-methyl-2-hexanone + $C_5H_{10}O_2$ isomer (tent.)	T
38	104	3-methylpyrrole (tent.)	83 ± 9
39	106	2,4-dimethylpyrrole	22 ± 2
40	107	ethylbenzene + ethylthiophene isomer	157 ± 17
40A	108	dimethylthiophene isomer	58 ± 57
41	109	m or p-xylene	255 ± 26
42	109	dimethylthiophene isomer	8 ± 1
43	110	3-heptanone	1 ± 0.5
43A	110	3-methylcyclohexanone	134 ± 17
44	111	2-heptanone	23 ± 3
45	112	styrene	175 ± 26
46	113	o-xylene	351 ± 239
46A	114	dimethylthiophene isomer	72 ± 16
47	114	dimethylpyridine isomer	106 ± 39
47A	115	C_9H_{18} isomer	33 ± 0
48	116	n-nonane	5 ± 0
48A	116	2,5-dimethylpyrrole	21 ± 2.6
48B	118	isopropylthiophene isomer	T
49	119	isopropylbenzene	5.6 ± 1
49A	119	C_9H_{18} + $C_{10}H_{22}$ isomers	T
50	120	2,5-dimethyl-2-cyclopentenone + $C_8H_{16}O$ isomer	T
51	122	2-ethylpyridine + ethylthiophene isomer	T
51A	123	$C_{10}H_{20}$ isomer	T
52	124	methylheptanone isomer + benzaldehyde	9 ± 2
53	125	n-propylbenzene	5.6 ± 3
54	125	m-ethyltoluene	66 ± 33
55	126	p-ethyltoluene	46 ± 24
56	127	cyanobenzene	57 ± 24
56A	128	$C_{11}H_{24}$ isomer	27 ± 3
57	129	phenol + 1,3,5-trimethylbenzene	NQ
58	130	trimethylthiophene isomer	8 ± 2
59	131	2-octanone	130 ± 24
60	132	benzofuran	287 ± 31
61	133	o-ethyltoluene	T
62A	136	n-decane	6 ± 2
63	138	1,2,4-trimethylbenzene	12 ± 6
63A	138	C_4-alkyl benzene isomer	13 ± 3
64	140	indan	153 ± 64
64A	141	indene	296 ± 37
65	142	cresol isomer	NQ
65A	143	C_4-alkyl benzene isomer	66.8 ± 17
65B	143	1,2,3-trimethylbenzene	62 ± 24

(continued)

Table C44 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
66	144	C_4-alkyl benzene isomer	T
67	147	$C_{10}H_{20}$ isomer	92 ± 21
68	148	C_4-alkyl benzene isomer	24 ± 10
68A	149	$C_{10}H_{12}$ isomer	28 ± 2
68B	149	C_4-alkyl benzene isomer	25 ± 5
69	150	$C_{10}H_{12}$ isomer	T
69A	150	cresol isomer	NQ
69B	151	methylbenzofuran + C_4-alkyl benzene isomers	20 ± 3
70	152	dimethylphenol isomer	NQ
71	152	2-methylbenzofuran	124 ± 24
72	153	*n*-undecane	117 ± 33
72A	154	dimethylphenol isomer	NQ
73	155	C_4-alkyl benzene isomer	8 ± 3
73A	155	C_4-alkyl benzene isomer	6 ± 3
73B	156	ethylphenol isomer	NQ
73C	158	dimethylphenol isomer	NQ
74	159	methylindan isomer	9 ± 2
74A	160	C_4-alkyl benzene + C_5-alkyl benzene isomers	33 ± 6
75	161	methylindene isomer	37.7 ± 13
75A	161	methylindan isomer	20 ± 10
76	162	methylindene isomer	7 ± 3
76A	162	dimethylphenol isomer	NQ
76B	163	C_5-alkyl benzene isomer	T
78	165	isopropylphenol isomer	NQ
78A	166	ethylphenol isomer	NQ
79	167	naphthalene	204 ± 107
79A	168	2,3-benzothiophene	T
79B	169	dimethylindan isomer	T
80	170	*n*-dodecane	117 ± 26
81	172	2,6-dimethylbenzofuran	T
82	173	dimethylbenzofuran isomer	T
82A	174	C_3-alkyl phenol isomer	NQ
83	175	dimethylindan isomer	T
85	179	methyldihydronaphthalene isomer	T
86	180	methyldihydronaphthalene + C_2-alkylindan isomers	T
87	183	dimethylindan isomer	T
87A	184	C_4-alkyl phenol isomer	NQ
87B	184	C_3-alkyl indan isomer	13 ± 6
88	185	β-methylnaphthalene	17 ± 13
88A	186	$C_{13}H_{26}$ isomer	40 ± 4
89	187	*n*-tridecane	22 ± 20
89A	187	C_3-alkyl indan isomer	T
89B	188	α-methylnaphthalene	4 ± 2
89C	190	C_4-alkyl phenol isomer	NQ
90A	193	C_6-alkyl benzene + C_5-alkyl phenol isomers	NQ
90B	194	C_4-alkyl phenol isomer	NQ
90C	197	biphenyl	T
91	200	$C_{14}H_{28}$ isomer	3.3 + 2
92	201	*n*-tetradecane	9 ± 5
92A	202	dimethylnaphthalene isomer	0.66 ± 0
93	205	dimethylnaphthalene isomer	7 ± 3
93A	207	dimethylnaphthalene isomer	T
93B	208	biphenylene	T
93C	209	ethylnaphthalene isomer	0.33 ± 0.33
93D	210	C_8-alkyl benzene isomer	T
93E	213	acenaphthene	4 ± 3
94	214	$C_{15}H_{30}$ isomer	17 ± 7
95	215	*n*-pentadecane	16 ± 10
95A	216	isopropylnaphthalene isomer	T
96A	222	isopropylnaphthalene isomer	T
98	228	*n*-hexadecane	42 ± 23
99	235	$C_{17}H_{36}$ isomer	3 ± 2
101	240	*n*-heptadecane	T
102	240	$C_{18}H_{38}$ isomer	T

Table C45. VOLATILE ORGANICS IN PRODUCED TAR (-17T) FROM WELL 7-8 IN SITU COAL GASIFICATION (LERC, ERDA)

Chromatographic Peak No.	Elution Temp. (°C)	Compound	ppm
1	55	CO_2	-
2A	59	acetaldehyde + propanol (tent.)	13 ± 5
2B	70	acetone	625 ± 300
3A	75	C_5H_{10} isomer + furan	T
3B	75	n-pentane	22 ± 5
3C	76	C_5H_8 isomer	T
3D	76	diethyl ether (tent.)	T
4	77	dichloromethane (BKG)	NQ
6	81	C_5H_8 isomer	T
6A	82	butanal (tent.)	NQ
6B	83	C_6H_{12} isomer + butanol (tent.)	T
6C	83	2-methylpentane	T
6D	84	isobutanal	T
6E	85	methyl ethyl ketone	300 ± 239
6F	86	C_6H_{12} isomer	T
7	86	hexafluorobenzene (e■)	
8	87	n-hexane	22 ± 10
9A	89	1-butanol	NQ
10	91	perfluorotoluene (e■)	
10A	92	methylcyclopentane	T
10B	93	n-butanal	2.2 ± 0.4
10C	94	C_6H_8 isomer	T
11	96	benzene	4683 ± 2000
11A	97	thiophene	96 ± 20
11B	98	C_7H_{16} isomer	T
11C	99	2-pentanone	380 ± 340
11D	100	2-methylbutanal	115 ± 25
12	101	C_7H_{14} isomer	T
12A	102	pentanal	60 ± 40
12B	102	C_7H_{12} + C_7H_{14} isomers	T
13	103	n-heptane	70 ± 30
13A	103	C_7H_{12} isomer	T
13B	104	C_7H_{14} isomer	T
14	105	C_7H_{12} isomer	3 ± 2.6
15	107	methylcyclohexane	T
15A	108	C_8H_{16} isomer	T
15B	108	4-methyl-2-pentanone	167 ± 134
15C	109	$C_6H_{12}O$ isomer	T
15D	110	C_7H_{12} isomer + 2-methyl-3-pentanone	T
15E	111	3-methyl-2-pentanone	83 ± 39
15F	113	C_7H_{12} isomer	T
16	114	toluene	920 ± 460
17	115	2-methylthiophene	219 ± 100
17A	116	3-methylthiophene	219 ± 100
17B	117	2-hexanone	300 ± 195
18	118	C_8H_{16} isomer	9 ± 3
18A	119	C_8H_{16} isomer	40 ± 10
18B	120	C_8H_{14} isomer	T
19	121	C_8H_{16} isomer	T
20	122	n-octane	400 ± 103
20A	123	C_8H_{16} + C_8H_{14} isomers	T
20B	124	C_8H_{14} isomer	T
21	124	C_8H_{16} + C_9H_{20} isomer	T
21A	125	C_9H_{18} isomer	T
22A	127	C_8H_{14} isomer	T
22B	127	$C_7H_{14}O$ isomer	T
23	128	C_9H_{20} isomer	42 ± 12
23A	128	C_8H_{16} isomer	12 ± 3
23B	129	C_8H_{14} + C_9H_{20} isomers	T
23C	129	C_8H_{16} isomer	T
24	130	ethylbenzene	T
24A	130	C_9H_{18} isomer	T
24B	131	C_8H_{14} isomer	T
24C	131	C_9H_{18} isomer	T
24D	132	C_9H_{16} isomer	T
25	132	m-xylene	605 ± 112
25A	133	C_8H_{16} isomer	10 ± 5
26	134	p-xylene	3389 ± 2247
26A	135	2,5-dimethylthiophene	15 ± 3
26B	137	2,3-dimethylthiophene	16 ± 6
27	138	styrene	460 ± 262
28	138	o-xylene	145 ± 1
28A	139	C_9H_{18} isomer	T
29	140	n-nonane	511 ± 20
29A	142	C_9H_{16} isomer	T
30	143	C_9H_{18} isomer	T
31	144	isopropylbenzene	193 ± 22
32	145	C_9H_{18} isomer	T
33	147	$C_{10}H_{22}$ isomer	T
33A	148	$C_{10}H_{20}$ isomer	T
34	149	$C_{10}H_{22}$ isomer	T
35	150	benzaldehyde + n-propylbenzene	20 ± 3.4
36	151	C_9H_{18} isomer	T
37	151	m-ethyltoluene + $C_{10}H_{20}$ isomer	3864 ± 1000
38	152	p-ethyltoluene + $C_{10}H_{22}$ isomer	3500 ± 600
38A	153	C_9H_{18} isomer	T
38B	153	$C_{10}H_{22}$ isomer	T
39	154	1,3,5-trimethylbenzene	622 ± 155
39A	155	C_9H_{18} isomer	T
39B	156	o-ethyltoluene	711 ± 424
39C	156	$C_{10}H_{20}$ isomer	T

(continued)

Table C45 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppm
39D	157	methylstyrene isomer	736 ± 235
40	158	1,2,4-trimethylbenzene	775 ± 244
41	159	*n*-decane	711 ± 313
42	161	$C_{10}H_{20}$ isomer	T
43	161	$C_{11}H_{22}$ isomer	T
43A	162	C_4-alkyl benzene isomer	T
44	162	1,2,3-trimethylbenzene	747 ± 489
44A	163	C_4-alkyl benzene isomer	NQ
45	163	$C_{11}H_{24}$ isomer	126 ± 24
46	164	indan	460 ± 31
47	166	indene	3158 ± 953
47A	166	C_4-alkyl benzene + $C_{11}H_{22}$ isomers	370 ± 70
47B	167	methylpropylbenzene isomer	152 ± 24
48	168	*n*-butylbenzene + dimethylethylbenzene + $C_{11}H_{22}$ isomer	64 ± 22
49	169	diethylbenzene isomer	21 ± 4.6
50	169	propyltoluene isomer	20 ± 7.4
50A	170	$C_{11}H_{24}$ + $C_{10}H_{20}$ isomers	10 ± 3
51	171	$C_{11}H_{24}$ isomer	T
51A	171	dimethylethylbenzene isomer	14 ± 2.6
52	172	dimethylethylbenzene + $C_{11}H_{22}$ isomers	T
52A	173	methylindan or $C_{10}H_{12}$ isomer	T
53	174	1-undecene	167 ± 79
54	175	vinylbenzaldehyde or methylbenzofuran isomer	63 ± 23
55	175	*n*-undecane + C_5-alkyl benzene isomer	T
56	176	2-methylbenzofuran	T
56A	177	C_5-alkyl benzene isomer	T
57	177	$C_{11}H_{22}$ isomer	T
58	178	tetramethylbenzene isomer	T
58A	179	$C_{12}H_{26}$ + $C_{10}H_{12}$ isomer	10 ± 52
59	180	dimethylindan + $C_{12}H_{26}$ isomers	53 ± 25
59A	180	C_5-alkyl benzene isomer	T
59B	181	tetramethylbenzene + $C_{11}H_{22}$ + $C_{12}H_{22}$ isomers	T
60	181	dimethylindan isomer	38 ± 10
60A	182	methylindan + C_5-alkyl benzene isomer	T
61	182	$C_{11}H_{22}$ isomer	4 ± 1
61A	183	$C_{12}H_{24}$ isomer	T
62	183	methylindene + methylindan isomers	69 ± 33
63	184	C_5-alkyl benzene isomer	24 ± 12
63A	184	methylindene isomer	T
64	185	C_5-alkyl benzene isomer	72 ± 30
64A	186	$C_{12}H_{26}$ isomer	57 ± 30
64B	186	$C_{12}H_{24}$ isomer	T
65	187	C_5-alkyl benzene isomer	T
65A	188	$C_{12}H_{24}$ + $C_{12}H_{22}$ isomers	T
65B	188	C_2-alkyl indan isomer	T
66	189	naphthalene	23684 ± 1353
66A	190	$C_{12}H_{24}$ isomer	75 ± 24
66B	191	C_2-alkyl indan isomer	T
66C	191	*n*-dodecane	715 ± 182
67	192	C_3-alkyl indan isomer	49 ± 20
68	194	4,7-dimethylbenzofuran + $C_{13}H_{28}$ isomer	T
69	194	C_6-alkyl benzene isomer	T
69A	196	C_6-alkyl benzene isomer	T
70	197	C_2-alkyl indan isomer	T
71	198	trimethylindan isomer	14 ± 6
71A	198	$C_{13}H_{26}$ isomer	2 ± 1
72	199	$C_{12}H_{16}$ isomer	20 ± 7.2
73	200	1-phenylhexane + methyldihydronaphthalene isomer	24 ± 5.6
74	201	$C_{13}H_{28}$ + C_6-alkyl benzene isomers	46 ± 30
75	201	methyldihydronaphthalene + $C_{11}H_{14}$ isomers	T
75A	202	$C_{14}H_{28}$ isomer	89 ± 28
76	202	$C_{14}H_{30}$ isomer	86 ± 21
77	203	C_3-alkyl indan isomer	T
78	204	C_3-alkyl indan isomer	T
78A	205	$C_{13}H_{26}$ isomer	79 ± 20
78B	206	C_3-alkyl indan + $C_{14}H_{28}$ isomers	11.2 ± 6
79	206	β-methylnaphthalene + *n*-tridecane	395 ± 124
79A	207	$C_{14}H_{28}$ isomer	T
79B	208	$C_{12}H_{16}$ isomer	T
80	209	α-methylnaphthalene	442 ± 80
81	211	$C_{12}H_{16}$ isomer	T
81A	212	C_7-alkyl benzene isomer	T
82	212	C_4-alkyl indan + $C_{14}H_{28}$ isomers	T
83	213	$C_{13}H_{26}$ isomer	14 ± 7.2
83A	214	C_4-alkyl indan isomer	35 ± 5.8
83B	215	1-phenylheptane	44 ± 12
84	215	$C_{14}H_{30}$ isomer	T

(continued)

Table C45 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppm	Chromato-graphic Peak No.	Elution Temp. (°C)	Compound
85	216	$C_{14}H_{26}$ isomer	85 ± 11			
86	217	$C_{15}H_{32}$ isomer	86 ± 12			
87	218	$C_{14}H_{26}$ isomer	84 ± 14			
87A	219	$C_{14}H_{28}$ isomer				
88	220	n-tetradecane	1700 ± 322			
89	221	$C_{15}H_{30}$ isomer				
90	224	$C_{15}H_{32}$ isomer	T			
91	226	C_7-alkyl benzene + $C_{15}H_{30}$ isomers	32 ± 5.2			
92	226	$C_{15}H_{32}$ isomer	T			
93	227	$C_{16}H_{32}$ isomer	82 ± 24			
93A	228	$C_{16}H_{34}$ isomer	T			
93B	229	$C_{15}H_{28}$ isomer	T			
94	230	$C_{16}H_{34}$ isomer	T			
95	231	$C_{15}H_{30}$ isomer	T			
96	232	n-pentadecane	53 ± 24			
96A	234	$C_{15}H_{30}$ isomer	T			
96B	235	$C_{15}H_{28}$ isomer	T			
97	236	$C_{15}H_{30}$ isomer	T			
97A	240	$C_{16}H_{32}$ isomer	T			
98	240	n-hexadecane	13 ± 6			
98A	240	$C_{16}H_{32}$ isomer	T			
98B	240	$C_{16}H_{34}$ isomer	T			
98C	240	$C_{16}H_{32}$ isomer	T			
98D	240	$C_{17}H_{32}$ isomer	T			
99	240	$C_{17}H_{34}$ isomer	7.4 ± 3.0			
100	240	n-heptadecane	5.6 ± 1.6			
100A	240	$C_{18}H_{38}$ isomer	T			
100B	240	$C_{17}H_{36}$ isomer	T			

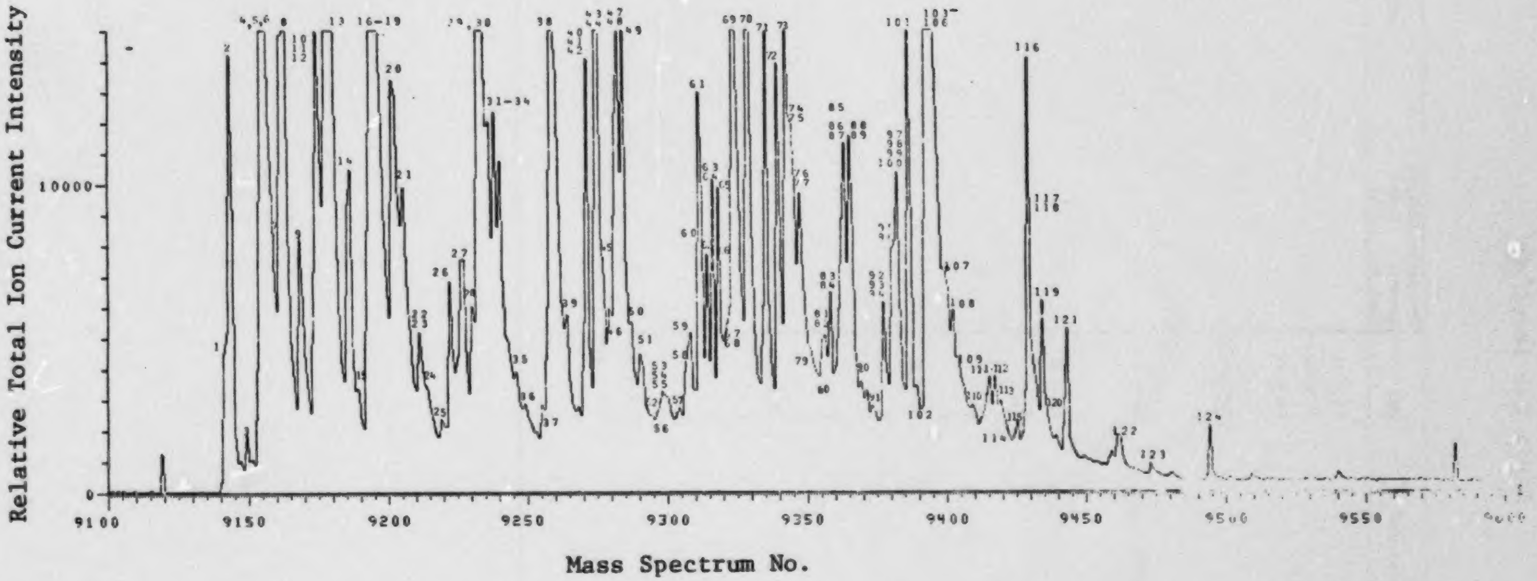


Figure C17. Profile of volatile organics in product water (-18L) during well 7-8 in situ coal gasification (LERC, ERDA).

Table C46. VOLATILE ORGANICS IN PRODUCED WATER (-18L) DURING WELL 7-8 *IN SITU* COAL GASIFICATION (LERC, ERDA)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
1	41	CO_2	-
3	45	acetaldehyde	360
4	46	acetonitrile	336
5	46	C_4H_{10} isomer	15
7	50	methyl-*n*-propyl ether	210
9	55	butadiene	36
10	58	C_5H_{12} isomer	49
11	59	perfluorobenzene (eS)	
12	60	C_7H_{14} isomer	62
14	63	perfluorotoluene (eS)	
15	64	C_6H_{14} isomer	71
17	68	benzene	315
18	68	C_6H_{12} isomer	69
20	69	C_6H_{14} isomer	T
21	72	C_6H_{14} isomer	31
22	73	C_6H_{14} isomer	6
23	73	C_7H_{16} isomer	2
24	74	C_7H_{12} isomer	1
25	76	C_7H_{14} isomer	T
26	80	C_7H_{16} isomer	15
27	81	pyrrole	300
28	83	C_7H_{12} isomer	7
29	85	C_7H_{14} isomer	6
30	86	toluene	297
31	88	methylthiophene isomer	115
32	89	methylthiophene isomer	96
33	90	C_7H_{16} isomer	26
34	92	dihydropyran	26
35	93	C_8H_{18} isomer	4
36	94	2-methylpyrrole	84
39	102	methylpyridine	162
40	104	methylpyridine	62
41	106	ethylbenzene	180
42	107	C_8H_{16} isomer	17
43	109	C_9H_{20} isomer	4
44	109	*m*-xylene	348
45	109	C_8H_{16} isomer	98
46	110	C_8H_{18} isomer	T
47	111	C_8H_{16} isomer	121
48	111	styrene or cyclooctatetraene	137
49	112	*o*-xylene	124
50	114	C_8H_{16} isomer	T
51	116	C_9H_{20} isomer	28
52	117	*o*-toluidine (tent.)	17
53	119	C_3-alkyl benzene	7
54	120	C_8H_{16} isomer	11
55	121	C_9H_{18} isomer	121
56	122	C_9H_{20} isomer	T
57	122	C_8H_{16} isomer	22
58	124	benzaldehyde	97
59	125	C_3-alkyl benzene isomer	32
60	126	C_9H_{18} isomer	28
61	127	C_3-alkyl benzene isomer	71
62	128	benzonitrile	97
63	129	C_3-alkyl benzene isomer	T
64	129	C_9H_{20} isomer	141
65	130	C_3-alkyl benzene isomer	129
66	131	C_9H_{18} isomer	77
67	132	phenol	NQ
68	133	benzofuran	180
69	133	C_3-alkyl benzene isomer	288
71	138	C_4-alkyl benzene isomer	94
72	140	indan	76
73	141	methylphenylacetylene isomer	T
74	143	cresol isomer	NQ
75	143	C_4-alkyl benzene isomer	T
76	144	methylphenylacetylene isomer	T
77	144	$C_{10}H_{20}$ isomer	T
78	145	C_4-alkyl benzene isomer	76
79	146	$C_{10}H_{20}$ isomer	89
80	147	cresol isomer	NQ
81	148	ethylstyrene isomer	6.8
82	148	C_4-alkyl benzene isomer	T
83	150	ethylstyrene isomer	439
84	151	C_4-alkyl benzene isomer	T
85	151	methylbenzofuran isomer	2.4
86	151	dimethylphenol isomer	NQ
87	151	methylbenzofuran isomer	4.8
88	153	methylbenzofuran isomer	T
89	153	C_4-alkyl benzene isomer	21
91	157	C_5-alkyl benzene isomer	33
92	159	dimethylstyrene isomer	3.2
93	159	C_5-alkyl benzene isomer	4
94	159	dimethylphenol isomer	NQ
95	160	unsat. C_5-alkyl benzene isomer	T
96	160	methylindene isomer	31
97	160	ethylstyrene isomer	32
98	161	C_4-alkyl benzene isomer	77
99	161	methylindene isomer	42
100	161	C_5-alkyl benzene isomer	5
101	163	C_3-alkyl phenol isomer	NQ
103	166	naphthalene	95

(continued)

Table C46 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
104	167	dimethylindan isomer	T
105	168	C_4-alkyl benzene isomer	37
106	168	C_3-alkyl phenol isomer	NQ
107	170	dimethylbenzimidazole (tent.)	NQ
108	171	dimethylindan isomer	T
109	172	C_3-alkyl phenol isomer	NQ
110	175	C_5-alkyl benzene isomer	3
111	177	dimethylindole (tent.)	28
112	180	$C_{11}H_{14}$ isomer	72
114	182	unsat. C_6-alkyl benzene isomer	4
115	183	$C_{11}H_{14}$ isomer	114
116	184	β-methylnaphthalene isomer	123
117	186	unsat. C_6-alkyl benzene	NQ
118	186	$C_{13}H_{28}$ isomer	NQ
119	187	α-methylnaphthalene isomer	29
120	190	unsat. C_6-alkyl benzene isomer	T
123	206	$C_{11}H_{24}$ isomer	

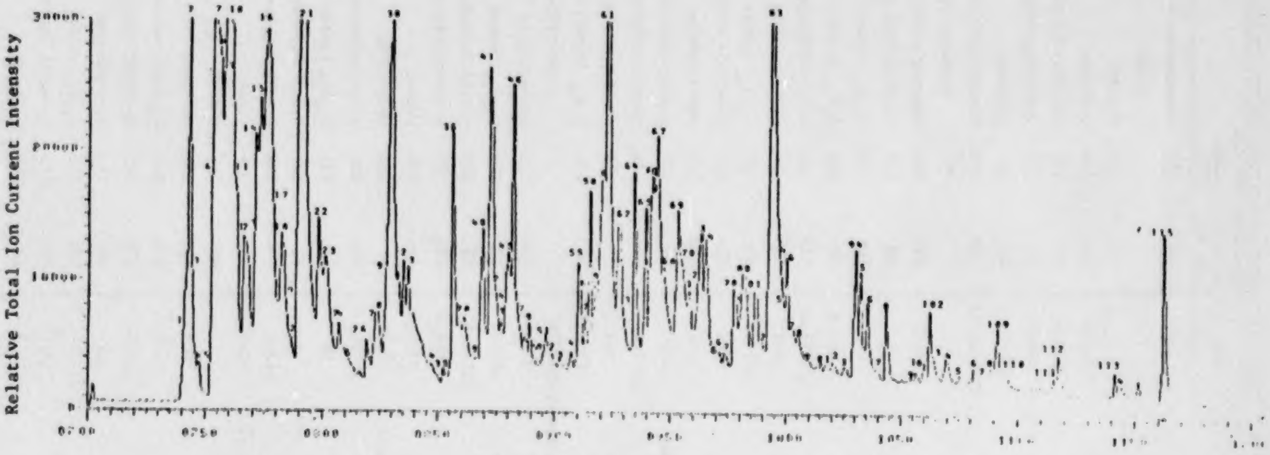


Figure C18. Profile of volatile organics in product water (-19L) from in situ coal gasification (LERC, ERDA).

Table C47. VOLATILE ORGANICS IN PRODUCED WATER (-19L) FROM WELL 7-8 *IN SITU* COAL GASIFICATION (LERC, ERDA)

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	ppb
1	41	CO_2	-
3	43	1-butene	T
4	44	*n*-butane	T
6	47	acetone	3340±50
7	48	ethanenitrile	223±18
8	48	dimethyl ether + diethyl ether	69±35
12	53	propanenitrile	619±155
13	56	methyl ethyl ketone	13230±1072
14	57	hexafluorobenzen (e■)	
15	58	*n*-hexane	20±17
17	60	isobutrylaldehyde (tent.)	T
18	62	perfluorotoluene (e■)	
20	64	3-methyl-2-butanone	9.6±4.6
21	66	benzene	4542±1262
21B	67	thiophene	69±23
22	69	2-pentanone	130±49
23	71	3-pentanone	79±3
24	74	C_7H_{16} isomer	17±1
24A	75	methylbutanenitrile isomer	43±0
25	76	$C_6H_{12}O$ isomer	13.3±0
25A	78	*N*-methylpyrrole	6±0
26	80	4-methyl-2-pentanone	17±1.67
27	82	pyrrole + 2-methyl-3-pentanone	1549±16
28	83	3-methyl-2-pentanone	31±8
29	84	*n*-pentanenitrile	461±92
30	85	toluene	2145±582
30A	86	2-methylthiophene	79±6.7
31	87	3-methylthiophene	92±9.3
32	88	cyclopentanone + 3-hexanone	55±13
33	89	2-hexanone	626±0
33A	91	sulfur compound	NQ
34	94	*n*-octane	T
35	97	$C_7H_{14}O$ isomer	167±9
37	100	methylcyclopentane + methylpyridine isomer	54±13
38	101	methylpyrrole isomer	6±5
38A	102	5-methyl-2-hexanone	26±0
38B	102	methylpyridine isomer	113±23
39	103	4-heptanone	10±7
39A	104	dimethylpyrrole isomer	T
40	105	ethylbenzene	53±11
40A	106	hexanenitrile	21±7
40B	106	dimethylthiophene isomer	11±0
41	107	*p*-xylene	232±60
42	108	dimethylthiophene isomer	17±2
43	109	3-heptanone	14±1
44	110	2-heptanone + ethylthiophene isomer	36.7±6.6
45	110	styrene	45.7±22
46	111	*o*-yxlene	132±14
47	112	dimethylthiophene isomer	7±4
48	113	2-ethylpyridine	19.3±2.6
49	114	*n*-nonane	4.3±2.3
49A	115	dimethylpyrrole + dimethylpyridine isomers	T
49B	116	dimethylpyridine isomer	T
50	117	isopropylbenzene isomer	3.0±6.7
50A	117	$C_{10}H_{22}$ isomer	19.7±1.0
51	118	C_9H_{18} isomer	10.3±1
51A	119	2-ethylcyclopentanone	T
52	120	ethylpyridine isomer	32±0.4
53	121	$C_{10}H_{22}$ isomer	8.3±2.3
53A	122	6-methyl-3-heptanone	32±8.6
53B	123	benzaldehyde	16±13
54	124	*n*-propylbenzene	5.0±0.7
55	125	*m*-ethyltoluene	53±5.7
56	125	*p*-ethyltoluene	32±1
57	126	C_9H_{18} isomer + 1,3,5-trimethylbenzene	176±44
57A	126	benzonitrile	28±2.7
58	127	$C_{11}H_{24}$ isomer	72±8.6
59	128	*o*-ethyltoluene	32±1
59A	129	trimethylthiophene isomer	2.7±1.7
60	130	phenol	NQ
61	131	benzofuran	237±27
61A	131	1,2,4-trimethylbenzene	120±13
63	135	$C_{10}H_{20}$ isomer	T
64	137	1,2,3-trimethylbenzene	130±14
64A	138	C_4-alkyl benzene isomer	42±27
65	139	indan	128±16
66	140	indene	273±59
67	141	*o*-cresol	NQ
67A	142	C_4-alkyl benzene isomer	28±2
67B	143	C_4-alkyl benzene isomer	7±4
68	143	acetophenone	11±0.3
68A	144	$C_{10}H_{20}$ isomer	5±0.7
68B	145	C_4-alkyl benzene isomer	5.7±2.6
69	146	*p*-cresol	NQ
69A	146	C_4-alkyl benzene isomer	19±3.6
70	147	methylindan isomer	1±0
70A	147	C_4-alkyl benzene isomer	19.7±2.7
71	148	methylindan isomer	78±24

(continued)

Table C47 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
71A	149	C_4-alkyl benzene isomer	2.3±1
71B	149	methylbenzofuran or C_9H_8O isomer	9±2
72	150	dimethylphenol isomer	NQ
73	151	2-methylbenzofuran	78±14
73A		C_5-alkyl benzene isomer	38±4.7
74	152	*n*-undecane	6±1
75	154	C_4-alkyl benzene isomer	T
76	155	C_4-alkyl benzene isomer	T
77	156	ethylphenol isomer	NQ
77A	157	C_5-alkyl benzene isomer	T
77B	158	dimethylindan isomer	1±0
78	158	dimethylphenol isomer	NQ
78A	159	C_5-alkyl benzene isomer	T
78B	159	methylindene isomer	33±2.7
79	160	methylindan isomer	8±4
79A	160	C_4-alkyl benzene isomer	28±6.3
80	161	methylindene isomer	18±1.7
80A	161	C_5-alkyl benzene isomer	T
80B	162	dimethylphenol isomer	NQ
81A	164	dimethylphenol isomer	NQ
82	165	C_3-alkyl benzene isomer	T
82A	166	dimethylphenol isomer	NQ
83	167	naphthalene	1796±22
84	168	benzothiophene isomer	90±9
85	169	dimethylindan isomer	15
85A	169	dimethylbenzofuran isomer	35±9
86	170	*n*-dodecane	11±1
86A	170	C_6-alkyl benzene isomer	8±3
87	171	4,7-dimethylbenzofuran	12±3
88	173	C_3-alkyl phenol isomer	NQ
89	175	dimethylindan isomer	3±2
89A	176	C_3-alkyl indan isomer	T
90	178	dimethylindan isomer	3±0.7
91	179	methyldihydronaphthalene isomer	T
92	180	methyldihydronaphthalene + C_2-alkyl indan isomers	5.3±
93	183	dimethylindan isomer	2±0.3
93A	184	C_3-alkyl indan isomer	6±3
94	185	α-methylnaphthalene	117±11
95	186	*n*-tridecane	11±1
95A	187	C_3-alkyl indan isomer	96±17
96	188	β-methylnaphthalene	57±6
97	190	C_3-alkyl indan isomer	T
98A	193	C_3-alkyl indan isomer	T
98B	195	C_4-alkyl indan isomer	T
99	197	biphenyl	6±0.3
100	198	$C_{12}H_{24}O$ isomer	4.6±2.3
101	200	$C_{14}H_{28}$ isomer	6.3±3
101A	201	ethylnaphthalene isomer	3±0.7
102	202	*n*-tetradecane	64±12
103	203	dimethylnaphthalene isomer	7.6±1
104	205	dimethylnaphthalene isomer	23±4
105	208	dimethylnaphthalene isomer	6±1
106	211	$C_{15}H_{32}$ isomer	12±5.6
106A	212	$C_{15}H_{30}$ isomer	3.6±1.3
107	213	2-tridecanone	1.7±1
108	214	$C_{15}H_{30}$ isomer	10.7±5.3
109	216	*n*-pentadecane	9.3±3
110	218	silane compound (BKG)	NQ
110A	226	tetradecanone isomer	14.7±2
111	227	$C_{16}H_{32}$ isomer	8.3±3.3
112	228	*n*-hexadecane	10.3±0.3
112A	240	$C_{15}H_{30}O$ isomer	T
113	240	$C_{17}H_{34}$ isomer	15.7±5.0
114	240	*n*-heptadecane	4.6±2.3

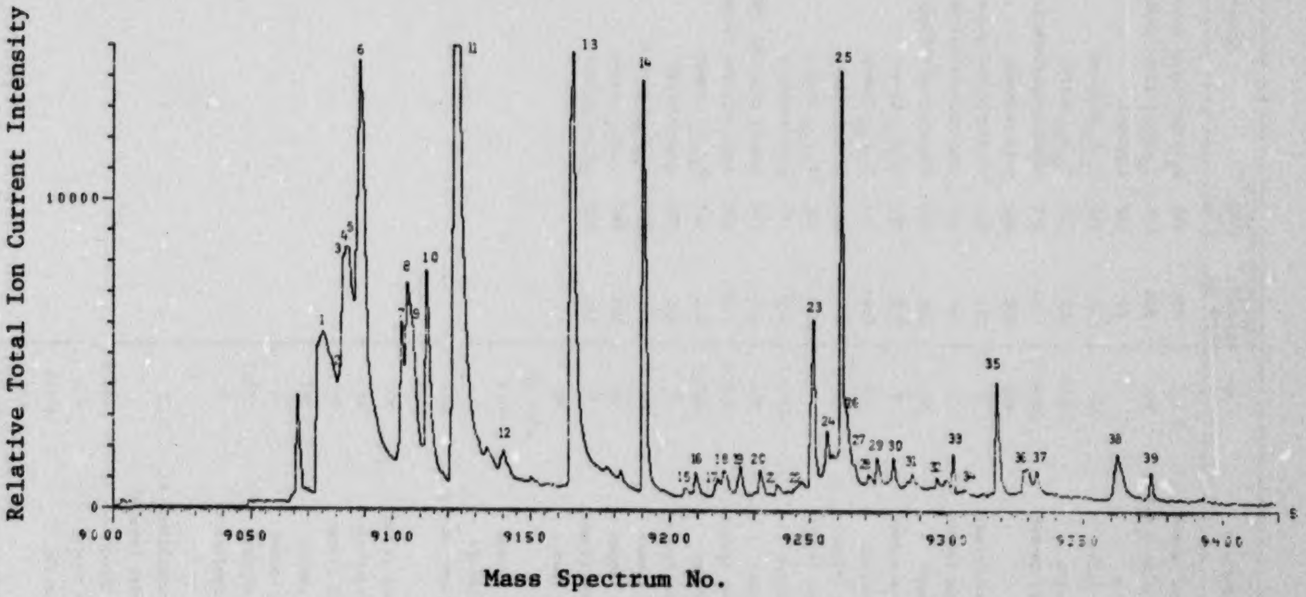


Figure C19. Profile of volatile organics in ground water sample from corehole #3 (-20L) after in situ coal gasification (LERC, ERDA).

Table C48. VOLATILE ORGANICS IN GROUND WATER (-20L) FROM COREHOLE #3 POST-*IN SITU* COAL GASIFICATION (LERC, ERDA)

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	ppb
1	57	acetaldehyde	2.50 ± 0.3
2	61	propenal	T
3	62	acetone	12.50 ± 3
4	63	diethyl ether	8.75 ± 0.9
6A	71	*n*-butanal	T
7	72	hexafluorobenzene (eS)	
8	73	*n*-hexane	2.82 ± 0.3
10	77	perfluorotoluene (eS)	
10A	78	methylcyclopentane	0.18 ± 0.11
11	82	benzene	150 ± 17
11A	84	cyclohexane	0.28 ± 0
11C	90	pentanal (tent.)	4.00 ± 0.9
12	91	*n*-heptane	0.25 ± 0
12A	96	methylcyclohexane	0.17 ± 0
13	103	toluene	2.76 ± 0.3
13A	109	4-methyl-2-pentanone	0.17 ± 0
13B	109	C_8H_{16} + C_8H_{18} isomers	0.77 ± 0.2
13C	111	C_8H_{18} isomer	0.23 ± 0.1
13D	112	*n*-octane	0.14 ± 0
15	123	ethylbenzene	0.12 ± 0
16	125	*m* or *p*-xylene	0.28 ± 0
16A	126	C_8H_{16} isomer	T
16B	128	C_9H_{20} isomer	T
16C	129	C_9H_{20} isomer	T
17	129	styrene	0.17 ± 0
17A	130	*o*-xylene + $C_7H_{14}O$ isomer	0.17 ± 0
18	130	C_9H_{20} isomer	0.45 ± 0.1
18A	131	C_9H_{18} isomer	0.26 ± 0
18B	132	heptanal isomer (tent.)	T
19	133	*n*-nonane	0.09 ± 0
19A	135	$C_7H_{14}O$ isomer	T
20	137	$C_{10}H_{22}$ isomer	T
20A	138	C_9H_{18} isomer	0.04 ± 0
20B	138	$C_{10}H_{22}$ isomer	T
20C	139	$C_{10}H_{20}$ isomer	T
21	140	$C_{10}H_{22}$ isomer	0.31 ± 0.1
21A	141	$C_{10}H_{20}$ + $C_{10}H_{16}$ (tent.) isomers	0.56 ± 0
21B	143	benzaldehyde	0.40 ± 0.1
21C	144	$C_8H_{16}O$ isomer	T
22	144	*m* or *p*-ethyltoluene	T
22A	145	$C_{10}H_{22}$ isomer	T
23	146	$C_{11}H_{24}$ isomer	5.01 ± 0.1
24	149	$C_{11}H_{24}$ isomer	1.50 ± 0.3
24A	150	$C_{10}H_{20}$ isomer + 1,2,4-trimethylbenzene	0.11 ± 0
26	152	*n*-decane	0.18 ± 0
27	154	$C_{11}H_{22}$ isomer	T
27A	156	1,2,3-trimethylbenzene	0.05 ± 0
28	156	$C_{11}H_{24}$ + C_4-alkyl benzene isomers	1.00 ± 0.2
29	158	$C_{12}H_{24}$ isomer	0.05 ± 0
29A	160	indene	0.18 ± 0
30	161	$C_{11}H_{24}$ isomer	0.20 ± 0
30A	162	C_4-alkyl benzene isomer	T
31	163	acetophenone	0.15 ± 0
31A	164	$C_{11}H_{24}$ isomer	0.55 ± 0.1
31B	166	C_4-alkyl benzene isomer	0.21 ± 0
31C	167	methylindan isomer	0.22 ± 0
31D	167	C_4-alkyl benzene isomer	T
32	169	$C_{10}H_{16}$ isomer	0.26 ± 0
32A	170	*n*-undecane	0.05 ± 0
33	172	$C_{10}H_{12}$ isomer	T
34	173	C_4-alkyl benzene isomer	T
34A	176	cresol isomer	NQ
34B	178	$C_{10}H_{20}O$ isomer	T
34C	179	dimethylphenol isomer	NQ
34D	179	methylindan + C_4-alkyl benzene isomers	0.07 ± 0
35A	183	dimethylphenol isomer	NQ
35B	183	$C_{12}H_{26}$ isomer	T
36	185	naphthalene	1.26 ± 0.1
37	187	*n*-dodecane	0.12 ± 0
37A	192	dimethylphenol isomer	NQ
38A	204	$C_{13}H_{28}$ isomer	0.04 ± 0
39A	217	*n*-tridecane	0.02 ± 0

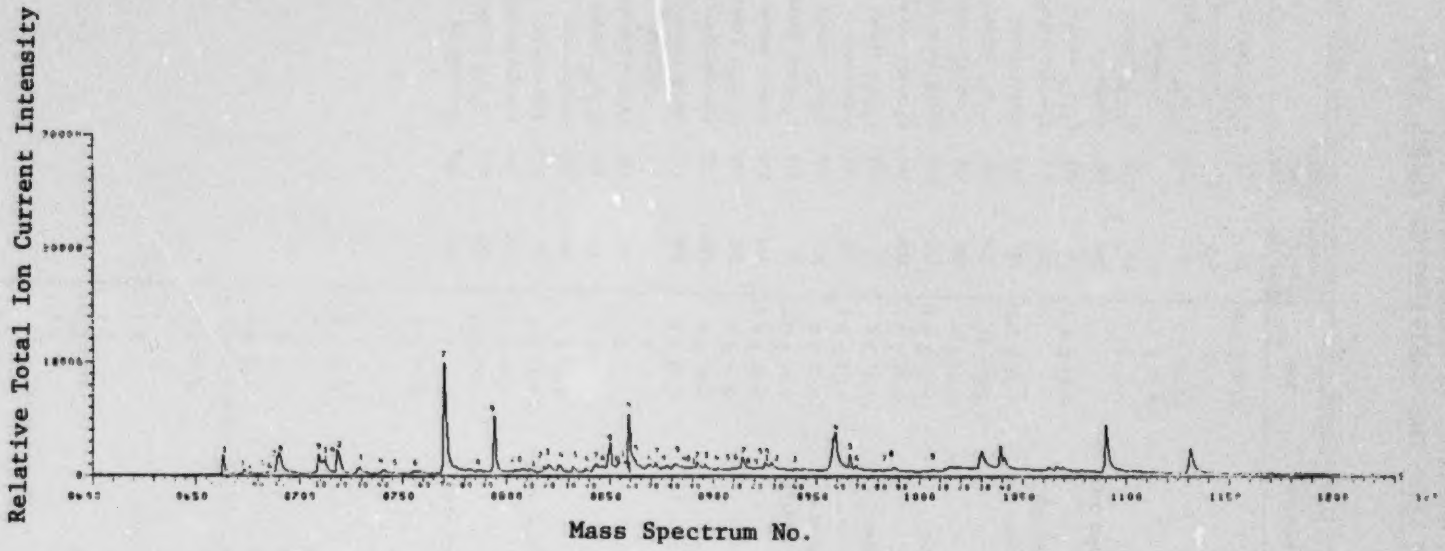


Figure C20. Profile of volatile organics in post-gasification water sample (-22L) from well #8, Hanna 1 (LERC, ERDA).

Table C49. VOLATILE ORGANICS IN POST-GASIFICATION (-21L) FROM WELL #1, HANNA #1 (LERC, ERDA)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb	Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
1	55	CO_2	NQ	47	170	n-undecane	0.11
2	57	propenal	NQ	48	176	cresol isomer	NQ
3	61	acetone	5.70	49	176	C_4H_7-benzene isomer	T
4	62	C_4H_{10} isomer	2.20	50	178	$C_{10}H_{20}O$ isomer	T
5	63	diethyl ether	9.92	51	179	C_5-alkyl benzene isomer	T
6	71	n-butanal	T	52	179	dimethyl phenol	NQ
7	73	perfluorobenzene (eS)		53	182	C_2-alkyl phenol	NQ
8	74	n-hexane	3.4	54	182	C_5-alkyl benzene isomer	T
9	77	perfluorotoluene (eS)		55	182	dimethylindan isomer	T
10	78	methylcyclopentane	0.55	56	184	dimethylindan isomer	T
11	84	benzene	3.22	57	194	C_4H_7-benzene isomer	T
12	85	cyclohexane	0.31	58	203	biphenyl	0.33
13	91	n-heptane	0.42	59	204	$C_{13}H_{28}$ isomer	0.06
14	96	methylcyclohexane	T	60	212	$C_{10}H_{22}$ isomer	T
15	106	toluene	6.75	61	217	n-tridecane	0.07
16	109	4-methyl-2-pentanone	0.22				
17	111	C_8H_{18} isomer	0.33				
18	112	n-octane	0.11				
19	115	C_7H_{16} isomer	T				
20	124	C_8H_{16} isomer	T				
21	129	ethylbenzene	1.20				
22	130	m- and p-xylene	3.92				
23	132	heptanal isomer	T				
24	133	C_7H_{14} isomer	T				
25	135	$C_7H_{14}O$ isomer	T				
26	136	C_8H_{18} isomer	T				
27	139	C_8H_{16} isomer	T				
28	140	C_8H_{14} isomer	T				
29	142	benzaldehyde	8.75				
30	143	C_3-alkyl benzene isomer	T				
31	145	C_8H_{16} isomer	T				
32	146	cyanobenzene	0.35				
33	149	$C_{11}H_{24}$ isomer	1.60				
34	149	C_3-alkyl benzene isomer	T				
35	150	$C_{11}H_{24}$ isomer	0.80				
36	151	phenol	NQ				
37	152	n-decane	0.39				
38	153	C_4-alkyl benzene isomer	T				
39	156	C_9H_{18} isomer	T				
40	159	C_4-alkyl benzene isomer	T				
41	160	indene	0.20				
42	161	$C_{11}H_{24}$ isomer	T				
43	162	C_4-alkyl benzene isomer	T				
44	163	acetophenone	T				
45	166	C_4-alkyl benzene isomer	T				
46	168	C_4-alkyl benzene isomer	T				

Table C50. VOLATILE ORGANICS IN POST-GASIFICATION WATER (-22L) FROM WELL #8, HANNA 1 (LERC, ERDA)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
1	52	CO_2	-
2	53	C_4H_8 isomer	NQ
3	56	acetaldehyde	T
4	58	C_4H_{10} isomer	1.38 ± 0.1
6	62	C_4H_{10} isomer	1.76 ± 0.3
9	74	perfluorobenzene (eI)	-
10	75	hexanol (tent.)	2.20 ± 0.1
12	79	perfluorotoluene (eI)	-
13	84	benzene	1.98 ± 1.2
15	93	C_7H_{16} isomer	5.30 ± 1.2
17	106	toluene	3.52 ± 2.5
18	115	C_7H_{16} isomer	T*
20	129	ethylbenzene	T
21	130	m- and p-xylene	3.42 ± 1.4
22	132	styrene and cyclooctatetraene	0.11 ± 0
23	133	C_7H_{14} isomer	T
24	136	C_8H_{18} isomer	T
25	139	C_8H_{16} isomer	T
26	140	C_8H_{14} isomer	T
27	141	benzaldehyde	7.50 ± 1.3
28	142	C_3-alkyl benzene isomer	T
29	145	C_8H_{16} isomer	T
30	146	cyanobenzene	0.25 ± 0
31	147	C_8H_{16} isomer	T
32	149	C_3-alkyl benzene isomer	T
33	149	C_3H_5-benzene isomer	T
35	151	phenol	NQ
36	153	C_4-alkyl benzene isomer	T
37	156	C_9H_{18} isomer	T
38	159	C_4-alkyl benzene isomer	T
39	161	C_3-alkyl benzene isomer	T
40	162	C_4-alkyl benzene isomer	T
41	164	C_4H_7-benzene isomer	T
42	166	C_4-alkyl benzene isomer	T
43	168	C_2-alkyl phenol isomer	NQ
44	172	C_4-alkyl benzene isomer	T
45	174	C_5-alkyl benzene isomer	T
46	176	C_4H_7-benzene isomer	T
48	179	C_5-alkyl benzene isomer	T
49	181	C_2-alkyl phenol isomer	NQ
50	182	C_5-alkyl benzene isomer	T
51	182	dimethylindan isomer	T
52	184	dimethylindan isomer	T
53	194	C_4H_7-benzene isomer	T
55	203	biphenyl	0.80 ± 0.2
57	212	$C_{10}H_{22}$ isomer	T

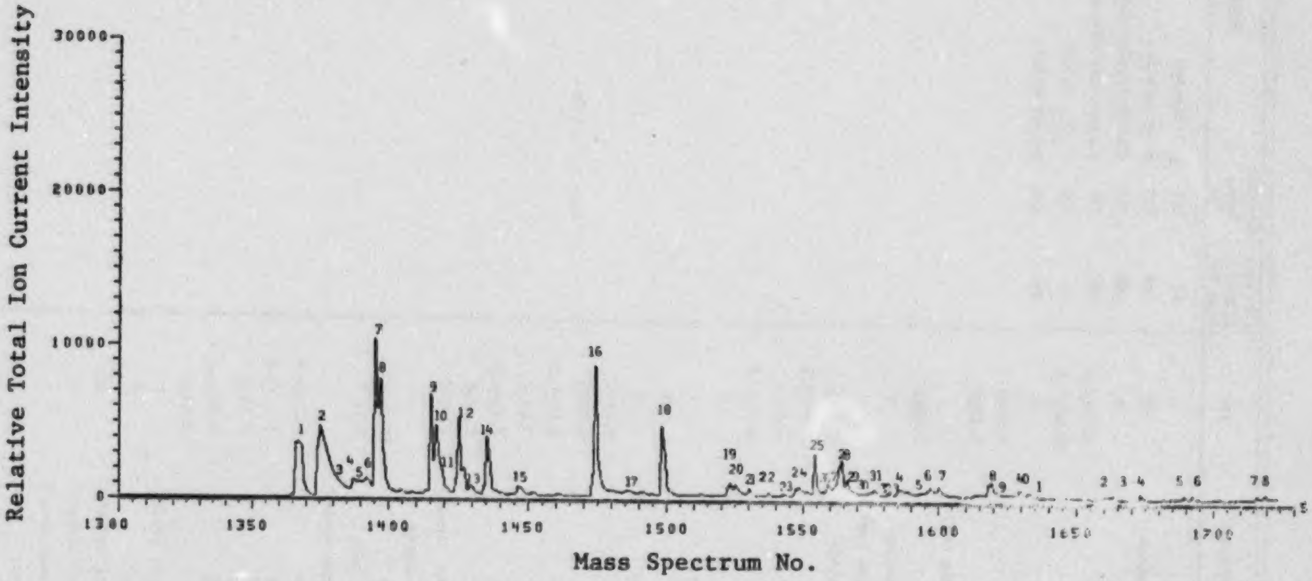


Figure C21. Profile of volatile organics in post-gasification water sample (-23L) from well WQ-1 after in situ coal gasification (LERC, ERDA).

Table C51. VOLATILE ORGANICS IN POST-GASIFICATION WATER (-23L) FROM WELL WQ-1 (LERC, ERDA)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
1	53	CO_2	-
1A	54	1-butene + n-butane	T
1B	55	2-butene	T
2	57	acetaldehyde	5.92±0.6
4A	64	acetone	10.42±3.3
5	65	n-pentane	T
6	66	diethyl ether	1.44±0.1
8A	77	butanal	0.22±0
9	78	perfluorobenzene (eI)	
10	79	n-hexane	0.58±0
11A	82	methyl ethyl ketone	T
12	83	perfluorotoluene (eI)	
12A	84	methylcyclopentane	0.18±0
14	88	benzene	0.64±0.1
15	93	n-heptane	0.05±0
16	103	toluene	8.82±0.9
17	116	n-octane	T
18A	120	furfural (tent.)	T
18B	121	ethylbenzene	T
18C	122	m or p-xylene	T
19	132	styrene	0.13±0
19A	133	o-xylene	0.05±0
20	133	C_9H_{20} isomer	2.00±0.5
21	135	n-nonane	0.14±0
22	139	$C_{10}H_{22}$ isomer	0.63±0.1
24	144	benzaldehyde	0.13±0
24A	145	n-propylbenzene (tent.)	0.05±0
24B	146	m or p-ethyltoluene	T
25	147	$C_{10}H_{22}$ isomer	12.26±3.3
25A	148	cyanobenzene (tent.) + methyl-styrene isomer	0.02±0
26	149	$C_{10}H_{22}$ isomer	4.29±1.8
27	151	$C_{10}H_{20}$ isomer	3.17±1.8
29	153	n-decane	0.32±0
31	158	$C_{11}H_{24}$ isomer	4.03±0.7
34	162	acetophenone	0.04±0
35	166	dimethylstyrene isomer	T
37	170	n-undecane	T
37A	176	dimethylphenol isomer	NQ
38A	181	dimethylphenol isomer	NQ
38B	181	C_4-alkyl benzene isomer	T
39	183	decanone isomer	T
40	184	$C_{12}H_{24}$ isomer	0.38±0.1
40A	185	ethylphenol isomer	NQ
41	186	n-dodecane	T
41A	196	ethylphenol isomer	NQ
43	201	n-tridecane	T
46A	218	n-tetradecane	T
46B	219	dimethylnaphthalene isomer	0.05±0
46C	221	dimethylnaphthalene isomer	0.02±0
47	227	$C_{15}H_{30}$ isomer	0.08±0
48	229	n-pentadecane	T

Table C52. VOLATILE ORGANICS IN POST-GASIFICATION WATER (-24L) FROM WELL #1, HANNA #2 (LERC, ERDA)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb	Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
1A	55	1-butene	T	28E	138	3-methyl-2-heptanone + $C_{10}H_{20}$ isomer	T
1B	55	n-butane	NQ	29	138	$C_{10}H_{22}$ isomer	0.13±0
2	56	acetaldehyde	5.20±1.7	29A	139	2-octanone	1.35±0.7
3	60	propanal	T	30	140	benzaldehyde	11.18±2.2
3A	61	acetone	T	31	140	n-propylbenzene + m-ethyl-toluene	T
3B	62	diethyl ether	0.56±0.1	31A	141	C_3-alkyl thiophene isomer	T
5	65	carbon disulfide	NQ	32	142	p-ethyltoluene	0.17±0
6	72	n-butanal	0.18±0	33	143	1,3,5-trimethylbenzene	0.12±0
7	73	hexafluorobenzene (eS)		34	144	$C_{10}H_{20}$ isomer	2.96±0.3
7A	74	n-hexane	1.33±0.3	34A	144	$C_{10}H_{22}$ isomer	0.57±0.1
9	77	perfluorotoluene (eS)		35	145	o-ethyltoluene	0.93±0.1
10	79	SO_2	NQ	35A	147	octanone isomer	0.36±0.1
12	82	benzene	13.41±1.1	35B	148	benzofuran	0.06±0
12A	84	thiophene (tent.)	T	36	148	1,2,4-trimethylbenzene	0.24±0
12B	88	$C_5H_{10}O$ isomer	T	38	150	n-decane	1.27±0.3
13	89	n-pentanal	T	39	152	phenol + $C_{10}H_{20}$ + C_3-alkyl thiophene isomers	1.15±0.2
14	91	n-heptane	0.13±0	40	153	1,2,3-trimethylbenzene	T
14A	92	C_7H_{14} isomer	0.12±0	40A	154	C_4-alkyl benzene isomer	0.55±0.1
14B	98	4-methyl-2-pentanone	0.18±0	41	156	indan	12.22±5.4
14C	100	$C_6H_{12}O$ isomer	T	42	157	C_4-alkyl benzene + $C_{11}H_{22}$ isomers	T
15	101	hexanal isomer	T	43	158	indene + C_4-alkyl benzene isomer	1.59±0.3
16	102	toluene	15.97±3.4	44-5	160	isobutylbenzene + diethyl-benzene isomer	T
16A	105	methylthiophene isomer (tent.)	T	46	162	C_4-alkyl benzene isomer	0.50±0.1
16B	107	2-methylpentanal	0.55±0	46A	163	C_5-alkyl benzene isomer	T
17	108	3-methylpentanal	0.55±0	47	163	tetramethylbenzene isomer	5.62±0.7
17A	109	n-hexanal + C_8H_{16} isomer	T	47A	164	diethylbenzene isomer	0.66±0.3
18	111	n-octane	0.26±0	47B	164	2-nonanone	NQ
19	113	$C_7H_{14}O$ isomer	T	48	165	methylindan isomer	1.25±0.7
20A	117	2-methylcyclopentanone	T	48A	165	C_4-alkyl benzene isomer	0.10±0
21	119	$C_7H_{12}O$ isomer	T	49	166	methylindan isomer	1.25±0.8
21A	121	heptanone isomer	T	50	167	$C_{11}H_{22}$ isomer	1.72±1.6
22	122	ethylbenzene	0.19±0	51	167	ethylheptanal isomer (tent.)	NQ
23	124	m or p-xylene	6.87±0.7	51A	168	methylbenzofuran or 2-methyl-benzimidazole + C_4-alkyl benzene + C_5-alkyl benzene isomers	16.75±4.78
24	127	2-heptanone	T	52	168	n-undecane	3.40±1.8
24A	127	dimethylthiophene isomer	T	52A	169	2-methylbenzofuran + C_4-alkyl benzene isomer	12.21±1.7
24B	128	styrene	0.12±0	53	170	C_5-alkyl benzene isomer	2.35±1.1
25	128	o-xylene	1.22±0.5				
26	130	C_9H_{18} isomer	0.14±0				
27	131	n-nonane	1.43±0.2				
27A	133	C_9H_{18} isomer	T				
28	135	isopropylbenzene	T				
28A	135	$C_{10}H_{22}$ isomer	0.18±0				
28B	136	$C_8H_{14}O$ isomer	0.14±0				
28C	136	octanone isomer	0.19±0				
28D	137	4-methyl-3-hepten-2-one	0.10±0				

(continued)

Table C52 (cont'd)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
54	171	tetramethylbenzene isomer	17.89±2.7
54A	173	dimethylindan isomer	7.78±0.8
55	173	C_5-alkyl benzene isomer	0.27±0.1
55A	174	methylindan isomer	T
56	175	C_5-alkyl benzene isomer	0.29±0.1
57	177	dimethylstyrene isomer	3.83±0.4
57A	178	C_5-alkyl benzene isomer + pentylbenzene	2.96±0.1
57B	179	C_5-alkyl benzene isomer	1.75±0.1
58	180	C_5-alkyl benzene + $C_{12}H_{26}$ isomers	0.57±0.1
59	181	C_6-alkyl benzene isomer	0.10±0
59A	182	decanone isomer	T
60	182	naphthalene	7.18±0.9
61	183	dimethylindan isomer	0.06±0
61A	184	dimethylindan isomer	7.02±1
62	186	*n*-dodecane	12.50±5.4
62A	187	C_3-alkyl indan isomer	T
62B	188	C_6-alkyl benzene isomer	T
63	188	dimethylbenzofuran or dimethyl-benzimidazole + $C_{13}H_{28}$ isomers	1.00±0.1
64	189	C_6-alkyl benzene + $C_{12}H_{16}$ isomers	0.57±0.1
66	192	$C_{12}H_{16}$ isomer	0.40±0.1
67	193	C_7-alkyl benzene isomer	0.65±0.1
67A	194	$C_{13}H_{18}$ isomer	0.10±0
68	195	C_6-alkyl benzene isomer	0.38±0.3
69	196	C_7-alkyl benzene isomer	0.41±0.3
69A	196	$C_{13}H_{28}$ isomer	11.00±1.0
70	198	$C_{14}H_{30}$ isomer	12.15±1.7
70A	199	$C_{12}H_{16}$ isomer	13.00±1.1
71	200	$C_{14}H_{30}$ isomer	4.50±1.7
71A	201	$C_{13}H_{26}$ isomer	4.77±0.6
72	202	*n*-tridecane + α-methylnaphthalene	
72A	204	$C_{12}H_{16}$ isomer	5.03±0.4
72B	205	$C_{13}H_{18}$ isomer	4.85±0.3
73	208	$C_{13}H_{18}$ isomer	0.50±0.1
73A	209	C_7-alkyl benzene isomer	0.12±0.1
74	209	$C_{13}H_{18}$ isomer	5.71±1.6
75	211	$C_{14}H_{30}$ isomer	6.74±2.3
75A	212	$C_{15}H_{32}$ isomer	8.15±2.0
76	213	$C_{15}H_{14}$ + $C_{13}H_{18}$ isomers	NQ
77	213	$C_{15}H_{32}$ isomer	NQ
79	216	$C_{14}H_{30}$ isomer	7.62±1.65
80	217	$C_{15}H_{30}$ isomer	2.76±1.0
80A	220	dimethylnaphthalene isomer	2.70±0.1
80B	222	$C_{15}H_{32}$ isomer	NQ
80C	223	$C_{15}H_{30}$ isomer	NQ
81	240	$C_{16}H_{34}$ isomer	NQ
82A	240	$C_{16}H_{34}$ isomer	NQ
83	240	$C_{17}H_{34}$ isomer	NQ
84	240	$C_{17}H_{36}$ isomer	NQ

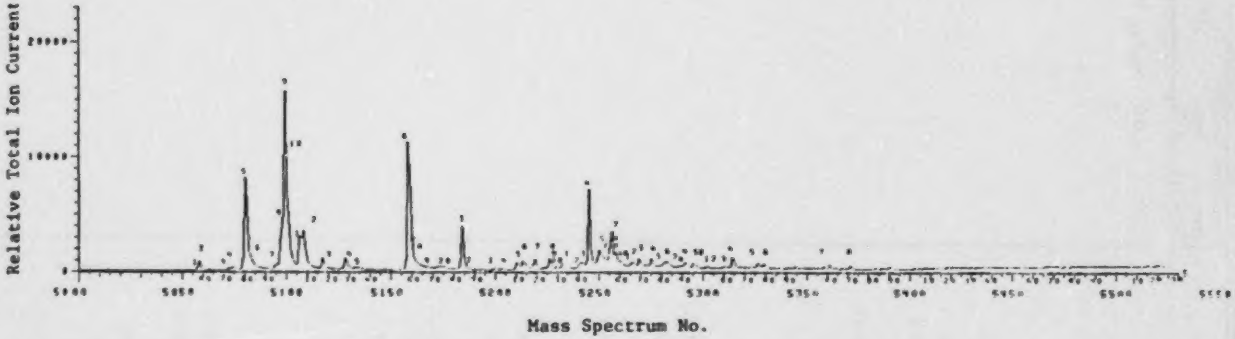


Figure C22. Profile of volatile organics in post-gasification water sample (-25L) from well #4, Hanna 11 (LERC, ERDA).

Table C53. VOLATILE ORGANICS IN POST-GASIFICATION WATER (-25L) FROM WELL #4 HANNA II (LERC, ERDA)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppb
1	49	$N_2 + O_2$	-
2	50	CO_2	-
6	63	C_4H_{10} isomer	T
7	69	methylpentane isomer	T
8	70	perfluorobenzene (eS)	
9	70	C_6H_{14} isomer	T
11	75	perfluorotoluene (eS)	
12	75	methylcyclopentane	1.60±0
13	80	benzene	1.09±0.3
15	92	C_7H_{16} isomer	T
16	102	toluene	11.24±1.31
17	103	C_7H_{16} isomer	T
18	107	C_8H_{18} isomer	T
22	120	C_8H_{16} isomer	T
23	122	C_2-alkyl benzene isomer	T
24	125	C_7H_{12} isomer	T
25	128	styrene	0.06±0
26	129	C_2-alkyl benzene isomer	0.20±0
27	132	C_8H_{16} isomer	0.22±0
28	136	C_9H_{20} isomer	0.30±0.1
29	137	$C_{10}H_{22}$ isomer	T
30	138	$C_{10}H_{20}$ isomer	T
31	139	$C_{10}H_{20}$ isomer	0.15±0
32	144	benzaldehyde	0.29±0
33	144	C_3-alkyl benzene isomer	T
34	146	$C_{11}H_{24}$ isomer	3.00±1.2
35	148	$C_{11}H_{24}$ isomer	1.10±0.6
36	149	$C_{11}H_{24}$ isomer	0.85±0.4
38	152	$C_{10}H_{22}$ isomer	T
39	152	$C_{11}H_{24}$ isomer	0.45±0.2
40	154	$C_{11}H_{22}$ isomer	T
41	156	C_3-alkyl benzene isomer	T
42	157	$C_{12}H_{24}$ isomer	T
43	158	$C_{12}H_{26}$ isomer	0.25±0.1
44	161	$C_{12}H_{26}$ isomer	0.23±0.1
45	162	C_4-alkyl benzene isomer	T
46	164	C_3-alkyl benzene isomer	0.16±0
47	165	C_3-alkyl benzene isomer	T
48	168	C_4-alkyl benzene isomer	T
49	169	C_5-alkyl benzene isomer	0.05±0
50	172	$C_{11}H_{24}$ isomer	T
51	174	C_5-alkyl benzene isomer	T
52	176	$C_{11}H_{20}$ isomer	T
53	179	C_5-alkyl benzene isomer	T
55	187	C_6-alkyl benzene isomer	T
56	188	$C_{12}H_{26}$ isomer	T
57	205	$C_{13}H_{28}$ isomer	T

APPENDIX D

SEMI-VOLATILE ORGANIC SUBSTANCES IN LIQUID AND SOLID EFFLUENTS FROM ENERGY-RELATED PROCESSES

		Page
Part I:	Samples from Oil-Shale Processing.	402
Part II:	Samples from Low Btu Gasification of Rosebud Coal. .	412
Part III:	Samples from *In Situ* Coal Gasification in Gillette, WY	426
Part IV:	Samples from *In Situ* Coal Gasification in Hanna, WY.	459

Table D1. SEMI-VOLATILE ORGANICS IN LIQUID SAMPLE FROM 150 TON RETORT *IN SITU* OIL-SHALE PROCESSING (LERC, ERDA)

Elution Temp. (°C)	Compound	ppb	Elution Temp. (°C)	Compound	ppb
97	*n*-butanal	NQ	133	$C_{13}H_{28}$ isomer	T
99	benzene	12	137	unknown	NQ
99	$C_5H_{10}O$ isomer	T	138	$C_{13}H_{26}$ isomer	T
100	isopropyl methyl ketone (tent.)	T	141	2-nonanone	T
101	*n*-pentanal	9	142	*n*-nonanal	75
103	C_9H_{18} isomer	T	143	$C_{14}H_{30}$ isomer	39
104	2-ethyl-1-hexanethiol (tent.)	29	148	$C_{14}H_{28}$ isomer	38
104	$C_{10}H_{20}$ isomer	19.8	152	*n*-decanal	48
105	toluene	T	155	2-decanone	T
107	*n*-hexanal	114	161	benzaldehyde	20
107	*n*-undecane	18	162	$C_{15}H_{30}$ isomer	33
110	C_9H_{18} isomer	T	176	acetophenone	13
112	$C_8H_{16}O$ isomer (tent.)	T	189	d_5-nitrobenzene (eS)	13
115	$C_{12}H_{26}$ isomer	5.4	215	cresol isomer	T
117	*n*-heptanal	165	216	phenol	237
119	cyclopentanone	57	222	C_2-alkyl phenol isomer	T
122	2-*n*-pentylfuran	T	223	dimethylphenol isomer	1011
123	$C_{12}H_{24}$ isomer	27	224	cresol isomer	720
128	2-octanone	T	228	C_2-alkyl phenol isomer	T
129	*n*-octanal	T	229	C_3-alkyl phenol isomer	T
131	cyclohexanone	T	230	dimethylphenol isomer	189
131	$C_{13}H_{28}$ isomer	T	231	dimethylphenol isomer	309
132	$C_{13}H_{26}$ isomer	T	234	ethylphenol isomer	321

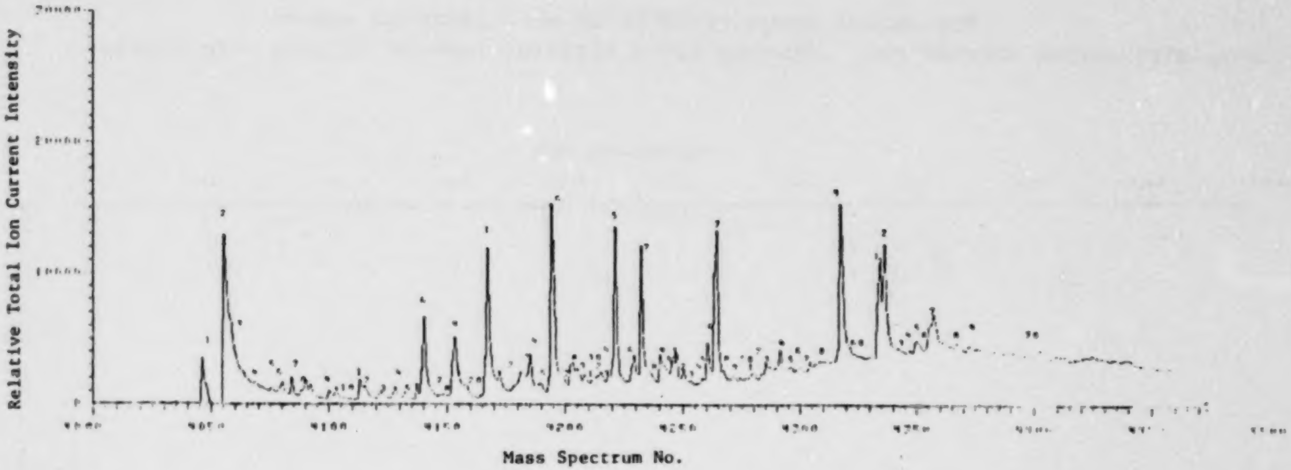


Figure D1. Profile of semi-volatile acid fraction from aqueous boiler blow-down sample obtained during in situ oil-shale processing.

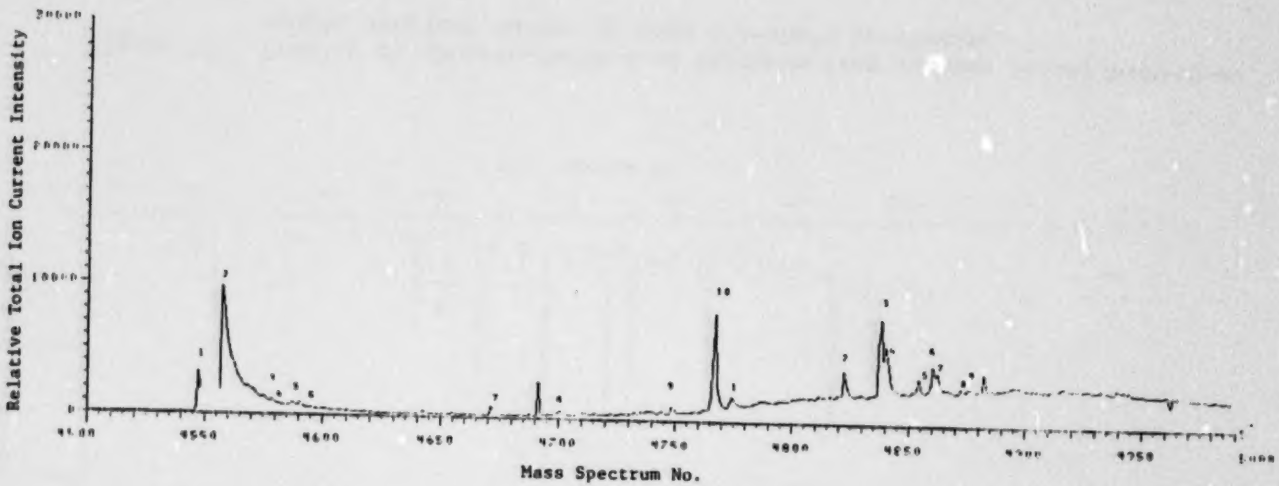


Figure D2. Profile of semi-volatile basic fraction from aqueous boiler blow-down sample obtained from in situ oil-shale processing.

Table D2. SEMI-VOLATILE ORGANICS IN AQUEOUS BOILER BLOW-DOWN SAMPLE FROM IN SITU OIL-SHALE PROCESSING (OCC)

Elution Temperature (°C)	Compound	ppb
93	CO_2	NQ
98	acetone	NQ
100	methyl ethyl ketone (tent.)	T
102	hydrocarbon (?)	NQ
104	n-butanal (tent.)	NQ
105	hydrocarbon (?)	NQ
107	hydrocarbon (?)	NQ
107	$C_5H_{10}O$ isomer + benzene (tent.)	T
108	n-pentanal (tent.)	T
109	toluene	T
109	α-methylbutyric acid	1.8
110	isopentanoic acid	4.2
112	aldehyde (tent.)	0.6
115	n-hexanal (tent.)	1.2
115	n-pentanoic acid	3.6
116	2-methylpentanoic acid	3.0
120	β-methylpentanoic acid	3.3
122	$C_7H_{14}O_2$ isomer	3.6
127	n-hexanoic acid	5.4
128	acid (?)	NQ
131	$C_7H_{14}O_2$ isomer	1.8
134	$C_7H_{14}O_2$ isomer (tent.)	4.2
136	acid (?)	NQ
140	n-heptanoic acid	54
144	acid (?)	NQ
146	2,4-dimethylheptanoic acid	52
149	unknown	NQ
154	n-octanoic acid	115
155	n-nonanal	9.6
156	3,5-dimethylheptanoic acid	4.8
160	acid (?)	NQ
163	3,5-dimethyloctanoic acid	34
165	acid (?)	NQ
168	n-nonanoic acid	132
170	$C_{11}H_{22}O_2$ isomer	2.4
170	$C_7H_{10}O$ isomer	1.2
170	n-decanal (tent.)	1.8
171	unknown	NQ
172	$C_8H_{12}O$ isomer	7.8
173	acid (?)	NQ
174	acid (?)	NQ
176	$C_7H_{10}O$ isomer (tent.)	1.8
176	C_6H_8O isomer (tent.)	10.8
178	$C_7H_{10}O$ isomer (tent.)	45.6
178	acid (?)	NQ
179	acid (?)	NQ
180	$C_8H_{12}O$ isomer	0.9
181	n-decanoic acid	123
186	3,5,5-trimethyl-2-cyclohexenone	10.2
186	acid (?)	NQ
186	benzoic acid	115
189	$C_8H_{12}O$ isomer	2.4
190	aldehyde (?)	NQ
191	acid (?)	NQ
193	cyclohexanedione (tent.)	1.2
193	n-undecanoic acid	1.8
195	$C_7H_{10}O_2$ isomer (tent.)	1.5
195	o-toluic acid	3.0
198	acid (?)	NQ
200	hydrocarbon (?)	NQ
200	m- or p-toluic acid	15.6
201	$C_7H_{12}O$ isomer (tent.)	1.2
202	d_5-nitrobenzene (e[illegible])	
205	$C_7H_{12}O$ isomer (tent.)	0.9
205	$C_8H_8O_2$ isomer	T
205	$C_8H_{14}O$ isomer	T
205	$C_9H_{16}O$ isomer (tent.)	T
205	unknown	NQ
205	$C_8H_{14}O$ isomer (tent.)	2.1
206	$C_8H_{14}O$ isomer	1.8
206	unknown	NQ
210	toluic acid isomer	2.7
212	β-phenylpropionic acid	1.2
215	2,5-dimethyltoluic acid	10.8
222	$C_{10}H_{12}O_2$ isomer	1.8
227	dimethylphenol isomer	3.0
228	phenol	459
228	cresol isomer	T
236	dimethylphenol isomer	552
238	cresol isomer	561
240	C_2-alkyl phenol isomer	19.2
240	C_3-alkyl phenol isomer (tent.)	T
240	dimethylphenol isomer	.0
240	ethylphenol isomer	17.4
240	C_2-alkyl phenol isomer	1.8
240	$C_{10}H_{16}O$ isomer	4.2
240	dimethylphenol isomer	125
240	C_3-alkyl phenol isomer	9
240	C_2-alkyl phenol isomer	231
240	$C_9H_{14}O$ isomer (tent.)	175

(continued)

Table D2 (cont'd)

Elution Temperature (°C)	Compound	ppb	Elution Temperature (°C)	Compound
240	$C_{10}H_{16}O$ isomer (tent.)	T		
240	C_3-alkyl phenol isomer	107		
240	$C_{11}H_{18}O$ isomer (tent.)	T		
240	C_3-alkyl phenol isomer	T		
240	C_3-alkyl phenol isomer	1.2		
240	alcohol (tent.)	NQ		
240	$C_{10}H_{16}O$ isomer (tent.)	17		
240	C_4-alkyl phenol isomer	8.4		
240	alkyl phenol (?)	37		

Table D3. SEMI-VOLATILE ORGANICS IN OMEGA-9 RETORT WATER FROM IN SITU OIL-SHALE PROCESSING PRIOR TO STORAGE AT 75°F (LERC, ERDA)

Elution Temperature (°C)	Compound	ppb
93	CO_2	NQ
95	acetaldehyde	NQ
97	ethyl formate	NQ
98	acetone	NQ
99	ethyl acetate	NQ
100	methyl ethyl ketone	T
101	dimethyl ether	NQ
101	hydrocarbon (?)	NQ
102	$C_{10}H_{22}$ isomer	T
106	$C_{11}H_{24}$ isomer (tent.)	1.5
108	n-pentanal	T
109	α-methylbutyric acid	24
110	isopentanoic acid	8
111	toluene	15
112	n-pentanoic acid	5
115	n-hexanal	T
116	2-methylpentanoic acid	4
120	β-methylpentanoic acid	6
122	n-hexanoic acid	38
131	$C_7H_{14}O_2$ (tent.)	NQ
135	n-heptanoic acid	79
137	methylpyridine	29
138	dimethylpyridine	77
141	acid (?)	NQ
142	C_7H_9N isomer	T
143	$C_8H_{11}N$ isomer	15
146	2,4-dimethylheptanoic acid	56
147	unknown	NQ
148	n-octanoic acid	14
148	hydrocarbon (?)	NQ
151	dimethylpyridine isomer	29
154	trimethylpyridine isomer	762
155	n-nonanal	4
155	$C_8H_{11}N$ isomer	621
156	2,4-dimethylheptanoic acid	41
157	alkyl pyridine isomer (?)	175
159	$C_9H_{13}N$ isomer	42
160	acid (?)	NQ
161	alkyl pyridine isomer	122
162	$C_7H_{10}O$ isomer	42
163	3,5-dimethyloctanoic acid	47
163	$C_8H_{12}O$ isomer	15
165	$C_9H_{14}O$ isomer	3
166	$C_9H_{13}N$ isomer	422
167	$C_8H_{11}N$ isomer	118
168	n-nonanoic acid	493
169	$C_9H_{14}O$ isomer	T
170	$C_7H_{10}O$ isomer	32
171	$C_8H_{12}O$ isomer	7
172	unknown	NQ
173	$C_8H_{11}N$ isomer	19
174	$C_9H_{14}O$ isomer (tent.)	26
175	hydrocarbon (?)	NQ
176	$C_{10}H_{15}N$ isomer (tent.)	T
177	$C_9H_{14}O$ isomer	T
178	acid (?)	NQ
178	cyanobenzene	32
178	$C_9H_{13}N$ isomer	T
179	$C_8H_{11}N$ isomer	19
180	$C_8H_{12}O$ isomer	3
181	δ-valerolactone	29
181	benzoic acid	227
183	acetophenone	10
185	aldehyde (?)	NQ
185	$C_9H_{13}N$ isomer	87
185	n-heptadecane	22
186	$C_9H_{13}N$ isomer	42
187	$C_{10}H_{15}N$ isomer	T
189	$C_9H_{13}N$ isomer (?)	T
190	aldehyde (?)	NQ
191	acid (?)	NQ
192	unknown (lactone ?)	NQ
193	hydrocarbon	T
194	toluic acid	21
195	d_5-nitrobenzene (e[illegible])	
198	n-octadecane	T
199	$C_{18}H_{36}$ isomer	5
200	hydrocarbon (?)	NQ
201	unknown	NQ
204	methylbenzoic acid isomer	T
204	$C_{18}H_{36}$ isomer	T
206	$C_{19}H_{38}$ isomer	5
208	C_2-alkyl aniline isomer	146
209	methylbenzoic acid isomer	
210	n-nonadecane	57
212	dimethylphenol isomer	51
212	β-phenylpropionic acid	4
214	C_2-alkyl aniline	T

(continued)

Table D3 (cont'd)

Elution Temperature (°C)	Compound	ppb
215	2,5-dimethytoluic acid	17
215	hydrocarbon (?)	NQ
216	aniline	497
217	C_3-alkyl phenol isomer	T
217	unknown	NQ
218	$C_8H_{11}N$ isomer	55
221	benzylamine	377
223	phenol	461
224	$C_8H_{11}N$ isomer	62
227	dimethylphenol isomer	15
228	$C_8H_{11}N$ isomer	T
229	quinoline	99
230	unknown	NQ
230	cresol isomer	779
230	$C_9H_{13}N$ isomer	T
230	dimethylnaphthalene isomer	199
232	ethylphenol isomer	69
233	methylquinoline isomer	41
234	$\underline{n}$-$C_{21}H_{44}$ isomer	38
234	$C_9H_{13}N$ isomer	11
237	C_2-alkyl phenol	T
238	C_2-alkyl phenol	T
240	C_2-alkyl quinoline (tent.)	T
240	dibenzofuran	29
240	fluorene	7
240	anthracene or phenanthrene	188
240	$C_{16}H_{14}$ isomer	T
240	$\underline{n}$-$C_{22}H_{46}$ (tent.)	T
240	C_2-alkyl quinoline	T

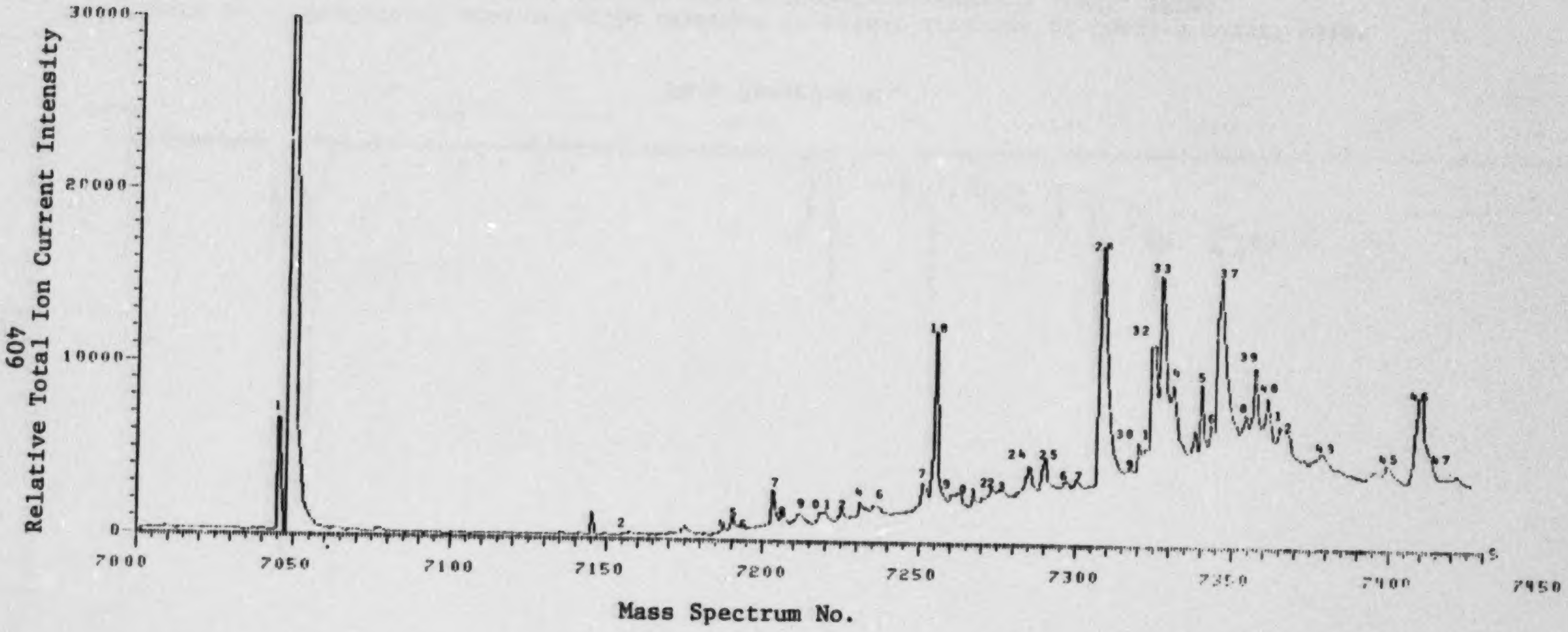


Figure D3 Profile of semi-volatile organics in neutral fraction of Omega-9 retort water (after incubation) from in situ oil-shale processing (LERC, ERDA).

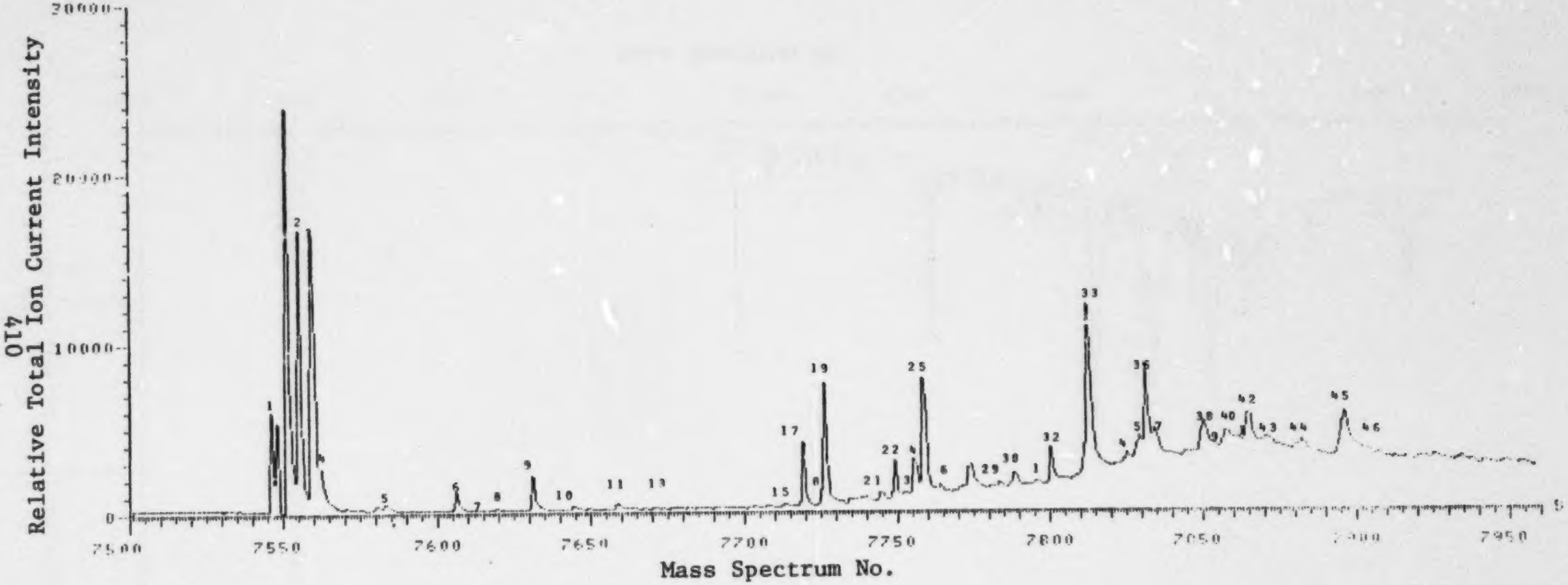


Figure D4 . Profile of semi-volatile organics in acidic fraction of Omega-9 retort water (after incubation) from in situ oil-shale processing (LERC, ERDA).

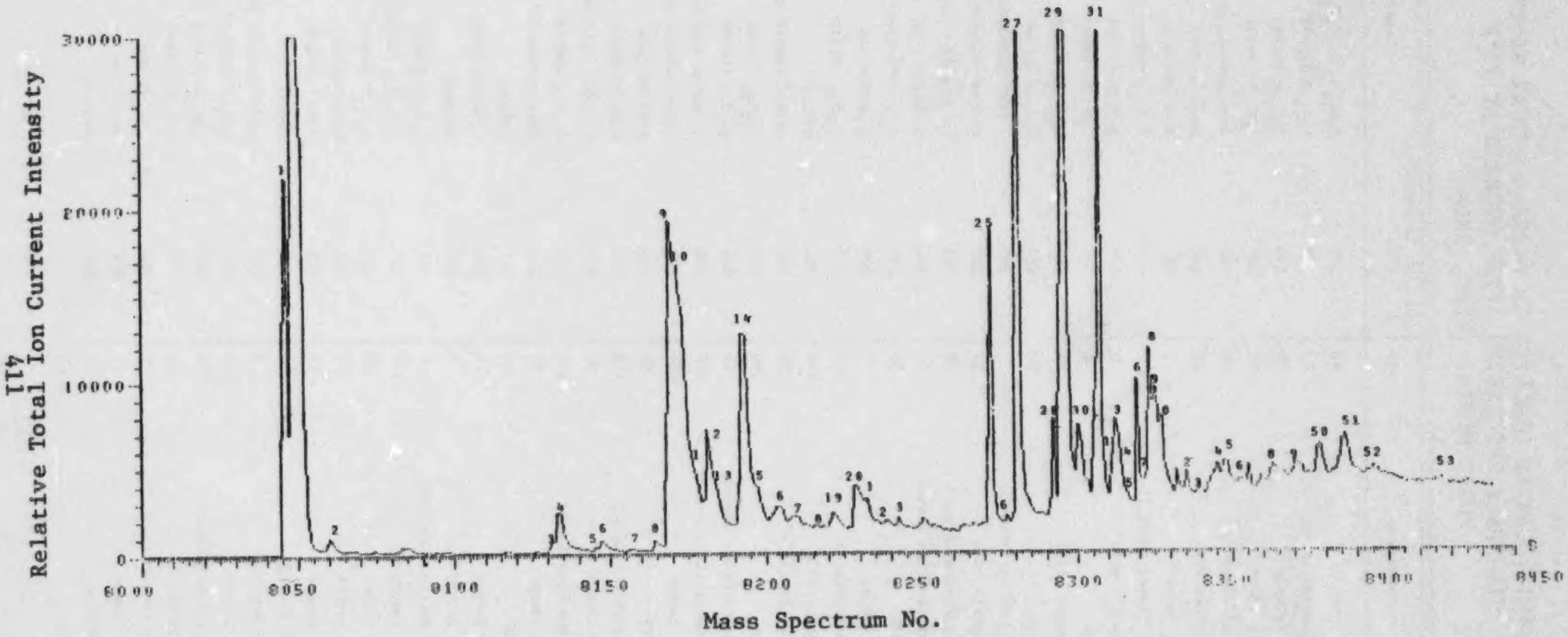


Figure D5 . Profile of semi-volatile organics in basic fraction of Omega-9 retort water (after incubation) from in situ oil-shale processing (LERC, ERDA).

Table D4. SEMI-VOLATILE ORGANICS IN OMEGA-9 RETORT WATER FROM *IN SITU* OIL-SHALE PROCESSING AFTER STORAGE AT 75°F FOR 2 MONTHS (LERC, ERDA)

Elution Temperature (°C)	Compound	ppb
92	CO_2	NQ
95	acetaldehyde (tent.)	NQ
97	ethyl formate	NQ
99	ethyl acetate	NQ
101	dimethyl ether	NQ
101	hydrocarbon (?)	NQ
102	$C_{10}H_{22}$ isomer	T
106	$C_{11}H_{24}$ isomer (tent.)	0.7
111	*n*-pentanoic acid	1.3
111	toluene	T
122	*n*-hexanoic acid	20
126	acid (?)	NQ
129	$C_7H_{14}O_2$ (acid) isomer	T
135	*n*-heptanoic acid	53
135	methylpyridine isomer	28
136	dimethylpyridine isomer	64
141	acid (?)	NQ
142	C_7H_9N isomer	T
143	$C_8H_{11}N$ isomer	9.6
148	*n*-octanoic acid	8.4
148	hydrocarbon (?)	NQ
148	unknown	NQ
151	dimethylpyridine isomer	13
153	trimethylpyridine isomer	555
154	$C_8H_{11}N$ isomer	406
157	acid (?)	NQ
157	alkyl pyridine isomer	176
159	$C_9H_{13}N$ isomer	34
161	alkyl pyridine isomer	118
162	$C_7H_{10}O$ isomer	33
162	acid (?)	NQ
163	$C_8H_{12}O$ isomer	13
165	$C_9H_{14}O$ isomer	T
165	$C_8H_{12}O$ isomer + unknown	T
166	$C_9H_{13}N$ isomer	383
167	$C_8H_{11}N$ isomer	95
169	$C_9H_{14}O$ isomer	T
170	$C_7H_{10}O$ isomer	29
170	$C_{10}H_{15}N$ isomer	15
171	$C_8H_{12}O$ isomer	3
173	$C_8H_{11}N$ isomer	8.4
174	$C_9H_{14}O$ isomer (tent.)	25
175	hydrocarbon (?)	NQ
176	$C_{10}H_{15}N$ isomer (tent.)	T
177	$C_9H_{14}O$ isomer	13
178	cyanobenzene	20
178	$C_7H_{14}O_2$ or $C_6H_{10}O_2$ isomer	57
178	$C_9H_{13}N$ isomer	T
179	$C_8H_{11}N$ isomer	16
180	$C_8H_{12}O$ isomer	2.4
181	δ-valerolactone	16
181	benzoic acid	111
183	acetophenone	T
183	$C_9H_{13}N$ isomer	79
185	*n*-heptadecane	T
185	$C_9H_{13}N$ isomer	35
187	$C_{10}H_{15}N$ isomer	T
189	$C_9H_{13}N$ isomer	T
190	*o*-methylbenzoic acid	4.2
192	unknown (lactone ?)	NQ
193	hydrocarbon (tent.)	T
194	*p*-toluic acid	30
195	d_5-nitrobenzene (e[illegible])	
198	*n*-octadecane	T
199	$C_{18}H_{36}$ isomer	10
201	unknown	NQ
204	methylbenzoic acid isomer	T
204	$C_{18}H_{36}$ isomer	T
206	$C_{19}H_{38}$ isomer	T
208	C_2-alkyl aniline isomer	154
209	methylbenzoic acid isomer	T
210	*n*-nonadecane	25
212	dimethylphenol isomer	34
214	C_2-alkyl aniline isomer	T
215	$C_{19}H_{38}$ isomer	T
215	hydrocarbon (?)	NQ
215	aniline	432
217	C_3-alkyl phenol isomer	T
217	unknown	NQ
218	$C_8H_{11}N$ isomer	46
219	*n*-$C_{19}H_{40}$ isomer	23
220	$C_8H_{11}N$ isomer	93
221	benzylamine	228
223	cresol isomer	94
223	phenol	293
223	methylaniline isomer	47
224	$C_8H_{11}N$ isomer	51
225	$C_9H_{13}N$ isomer (tent.)	43
227	$C_8H_{11}N$ isomer	34
228	$C_8H_{11}N$ isomer	T
229	quinoline	71
229	unknown	NQ

(continued)

Table D4 (cont'd)

Elution Temperature (°C)	Compound	ppb	Elution Temperature (°C)	Compound
229	$\underline{n}$-$C_{20}H_{42}$ isomer	T		
230	$C_{15}H_{12}$ isomer	69		
230	$C_9H_{13}N$ isomer	43		
230	dimethylnaphthalene isomer	189		
230	ethylphenol isomer	68		
231	methylquinoline isomer	70		
234	$\underline{n}$-$C_{21}H_{44}$ isomer	34		
234	$C_9H_{13}N$ isomer	9		
234	C_2-alkyl phenol isomer	T		
235	C_3-alkyl phenol isomer	9		
235	$C_8H_{11}N$ isomer	8.4		
237	C_2-alkyl phenol isomer	14		
237	methylquinoline isomer	T		
238	C_3-alkyl phenol isomer	T		
238	C_2-alkyl phenol isomer	T		
239	C_2-alkyl phenol isomer	337		
240	C_2-alkyl quinoline isomer (tent.)	T		
240	C_3-alkyl phenol isomer	17		
240	cresol isomer	35		
240	C_3-alkyl phenol isomer	17		
240	C_3-alkyl naphthalene isomer	9		
240	C_3-alkyl phenol isomer	46		
240	tri-sec-butyl phenol isomer (tent.)	17		
240	C_3-alkyl phenol isomer	8.4		
240	C_3-alkyl naphthalene isomer	2.4		
240	dibenzofuran	10		
240	fluorene	3		
240	anthracene or phenanthrene	154		
240	$C_{13}H_{10}O$ (hydroxyfluorene ?)	47		
240	$C_{16}H_{14}$ isomer	T		
240	$\underline{n}$-$C_{22}H_{46}$ (tent.)	T		
240	C_2-alkyl quinoline isomer	T		
240	C_2-alkyl quinoline isomer	T		

Table D5. SEMI-VOLATILE ORGANICS IN AQUEOUS CONDENSATE (-1L) FROM LOW BTU GASIFICATION OF ROSEBUD COAL (MERC, ERDA)

Elution Temperature (°C)	Compound	ppb
93	CO_2	NQ
100	acetaldehyde	NQ
100	n-propanal	NQ
100	ethyl formate	0.8
101	ethyl acetate	1.2
101	n-butanal	NQ
102	n-nonane	3.1
103	C_9H_{20} isomer	T
104	benzene	275
105	n-decane	0.6
106	hydrocarbon	T
111	toluene	T
113	$C_{11}H_{24}$ isomer	T
114	unknown	NQ
119	ethylbenzene	T
120	m or p-xylene	1.2
123	$C_7H_{14}O$ isomer	T
124	n-dodecane	3.0
124	o-xylene	3.6
126	cyclopentanone	T
127	2-methylcyclopentanone	0.7
127	n-propylbenzene	T
129	ethyltoluene isomer	6.6
130	$C_{12}H_{24}$ isomer	T
134	styrene	T
134	C_3-alkyl benzene isomer	T
135	C_4-alkyl benzene isomer	0.6
137	n-tridecane	7.8
137	C_3-alkyl benzene isomer	1.2
139	$C_{13}H_{26}$ isomer	T
140	$C_{13}H_{26}$ isomer	T
141	C_4-alkyl benzene isomer	T
143	$C_{13}H_{26}$ isomer	T
144	$C_{14}H_{30}$ isomer	T
145	C_3-alkyl benzene isomer	1.8
146	$C_7H_{10}O$ isomer (tent.)	T
147	C_4-alkyl benzene isomer	T
148	methylstyrene isomer	T
148	$C_7H_{10}O$ isomer (tent.)	T
150	n-tetradecane + C_9H_{10} isomer	16.2
152	C_4-alkyl benzene isomer (tent.)	T
154	ethylstyrene isomer (tent.)	T
155	n-butylbenzene	T
157	$C_{13}H_{26}$ isomer	T
158	C_5-alkyl benzene isomer	T
158	C_4-alkyl benzene isomer	0.8
163	n-pentadecane	1.2
164	$C_{10}H_{12}$ isomer	T
164	saturated ketone	T
165	indene	210.8
165	C_4-alkyl benzene isomer	2.4
166	C_5-alkyl benzene isomer	T
166	$C_8H_{12}O$ isomer	T
167	benzofuran + $C_{10}H_{12}$ isomer	129.6
168	$C_{11}H_{14}$ + $C_9H_{14}O$ isomers	T
168	phenylhexane isomer	1.2
171	C_6-alkyl benzene isomer	1.5
173	ketone (?)	NQ
175	ketone (?)	NQ
177	n-hexadecane	1.2
178	1-methyl-1H-indene	T
179	2-methylbenzofuran	1.6
180	methylindene isomer	T
181	cyanobenzene	7.8
182	phenylheptane isomer	T
184	ketone (?)	NQ
185	$C_{11}H_{14}$ + C_7-alkyl benzene isomers	T
187	acetophenone	9.0
188	1-ethylindan	T
190	$C_{11}H_{14}$ isomer	T
191	$C_{10}H_{14}$ isomer	T
192	methyl-1,2-dihydronaphthalene isomer	T
192	$C_{13}H_{18}$ isomer	T
193	unknown	NQ
193	dimethylbenzofuran isomer	T
194	methyl-1,2-dihydronaphthalene isomer	T
196	phenyl-n-octane	T
197	$C_{11}H_{22}$ isomer	T
198	d_5-nitrobenzene (eI)	
199	naphthalene	454
202	methylacetophenone isomer	4.2
203	$C_{12}H_{16}$ isomer	T
206	2,3-benzothiophene	1.8
207	$C_{12}H_{16}$ isomer	T
212	methylnaphthalene isomer	715.6
213	$C_{13}H_{18}$ isomer	3
216	dimethylphenol isomer	T
216	methylnaphthalene isomer	117.4

(continued)

Table D5 (cont'd)

Elution Temperature (°C)	Compound	ppb	Elution Temperature (°C)	Compound
219	tetramethylindanone (tent.)	1.8		
221	methylethylphenol isomer	2.1		
222	ethylnaphthalene isomer	T		
224	dimethylnaphthalene isomer	T		
224	cresol isomer	147		
225	phenol	10		
225	C_3-alkyl phenol isomer	1.3		
226	biphenyl	T		
228	dimethylnaphthalene isomer	2.4		
229	C_4-alkyl phenol isomer	T		
230	indan-1-one (tent.)	T		
230	C_3-alkyl phenol isomer	0.6		
231	ethylphenol isomer + C_2-alkyl naphthalene	T		
231	dimethylphenol isomer	T		
233	C_4-alkyl phenol isomer	30		
233	cresol isomer	186		
234	cresol isomer	129		
235	C_3-alkyl naphthalene isomer	T		
236	C_5-alkyl phenol isomer	25		
236	C_2-alkyl phenol isomer	T		
237	C_3-alkyl phenol isomer	T		
238	methylbiphenyl isomer	T		
239	C_3-alkyl phenol isomer	1.7		
240	C_3-alkyl naphthalene	0.6		
240	dimethylphenol isomer	1.3		
240	C_3-alkyl phenol isomer	T		
240	ethylphenol isomer	28.8		
240	dimethyl phenol	70		
240	ethylphenol isomer	9.6		
240	C_3-alkyl phenol isomer	T		
240	C_2-alkyl phenol isomer	T		
240	acenaphthene	T		
240	C_4-alkyl phenol isomer	T		
240	biphenylene	0.9		
240	sec-butyl phenol isomer	1.2		
240	trimethylnaphthalene isomer	1.6		
240	dibenzofuran	1.8		
240	fluorene	1.7		

Table D6. SEMI-VOLATILE ORGANICS IN AQUEOUS CONDENSATE (-2L) FROM LOW BTU GASIFICATION OF ROSEBUD COAL (MERC, ERDA)

Elution Temperature (°C)	Compound	ppb
92	CO_2	NQ
95	acetaldehyde	NQ
97	acetone	NQ
97	ethyl formate	T
99	*n*-butanal	NQ
100	methyl ethyl ketone	T
100	ethyl acetate	NQ
101	hydrocarbon (?)	9
102	dimethyl ether	NQ
103	*n*-nonane (tent.)	T
103	benzene	200
104	*n*-pentanal	NQ
105	*n*-decane	10
106	$C_6H_{12}O$ isomer	T
106	hydrocarbon (?)	T
109	toluene	180
110	*n*-undecane	15
111	*n*-hexanal	T
113	$C_{11}H_{22}$ isomer	T
114	ethylbenzene	T
115	xylene isomer	T
116	*n*-dodecane	145
119	$C_{12}H_{24}$ isomer	T
119	C_7H_{14} isomer	234
121	*n*-propylbenzene	18
122	ethyltoluene isomer	T
123	$C_6H_{10}O$ isomer (tent.)	T
124	*n*-tridecane	396
126	$C_{13}H_{26}$ + C_4-alkyl benzene isomers	T
126	trimethylbenzene isomer	T
127	$C_{13}H_{26}$ isomer	T
129	trimethylbenzene isomer	7.5
130	$C_{14}H_{28}$ isomer	T
131	C_4-alkyl benzene isomer	T
131	2-octanone	19.5
132	C_4-alkyl benzene isomer	T
132	*n*-butylbenzene	T
133	$C_{13}H_{24}$ isomer	T
134	C_4-alkyl benzene isomer	T
136	methyl-*n*-propylbenzene isomer	T
138	trimethylbenzene isomer	T
138	*n*-tetradecane	T
140	C_4-alkyl benzene isomer	T
141	C_4-alkyl benzene isomer	T
143	$C_7H_{10}O$ isomer	T
143	indan	10.5
144	C_5-alkyl benzene isomer	T
145	$C_9H_{18}O$ isomer	19.5
146	methylindan isomer	T
146	*n*-pentylbenzene	T
147	$C_{15}H_{30}$ isomer	T
148	C_6H_8O isomer	9
148	C_5-alkyl benzene isomer	T
150	C_4-alkyl benzene isomer	T
150	C_5-alkyl benzene isomer	T
152	C_4-alkyl benzene isomer	T
157	$C_7H_{10}O$ isomer	T
158	methylindan isomer	T
159	C_6-alkyl benzene isomer	T
160	$C_{10}H_{20}O$ + C_4-alkyl benzene isomers	63
160	indene	108
162	methylindan isomer	T
163	benzofuran	T
163	$C_{15}H_{32}$ isomer (tent.)	T
164	C_8H_{12} isomer	27
165	$C_{11}H_{14}$ isomer	T
165	C_6-alkyl benzene isomer	T
167	benzaldehyde	T
170	$C_7H_{10}O$ isomer	54
171	$C_{12}H_{16}$ isomer	18
172	$C_8H_{12}O$ isomer	10.5
173	$C_{11}H_{14}$ isomer	T
174	methylindene isomer	9
175	methylbenzofuran isomer	21
177	methylindene isomer	18
178	cyanobenzene	T
178	phenyl-*n*-heptane	T
179	$C_{12}H_{16}$ isomer	T
180	$C_{11}H_{14}$ isomer	54
183	acetophenone	18
184	C_2-alkyl indan isomer	12
185	C_3-alkyl indan isomer	T
186	$C_{11}H_{12}$ isomer	T
186	C_3-alkyl indan isomer	9
188	$C_{11}H_{12}$ isomer	T
188	$C_{13}H_{18}$ isomer (tent.)	T
190	dimethylbenzofuran isomer (tent.)	27
190	$C_{11}H_{12}$ isomer	28
193	$C_{11}H_{12}$ isomer	10

(continued)

Table D6 (cont'd)

Elution Temperature (°C)	Compound	ppb
193	phenyl-n-octane	T
194	C_8-alkyl benzene isomer	T
196	d_5-nitrobenzene (eB)	
197	naphthalene	1410
197	alkyl indan isomer	T
199	$C_{12}H_{16}$ isomer	11
200	C_9-alkyl benzene isomer	9
202	2,3-benzothiophene	189
203	$C_{12}H_{16}$ isomer	T
205	$C_{14}H_{20}$ isomer	T
208	methylnaphthalene isomer	870
209	$C_{13}H_{18}$ isomer	465
211	dimethylphenol isomer	T
213	methylnaphthalene isomer	414
216	pentamethylindan isomer	T
216	C_3-alkyl phenol isomer	54
217	C_5-alkyl indan isomer	T
219	ethylnaphthalene isomer	11
221	cresol isomer	T
221	dimethylnaphthalene isomer + phenol	288
222	C_3-alkyl phenol isomer	144
223	o-cresol	2535
223	biphenyl	9
223	dimethylnaphthalene isomer	345
224	dimethylnaphthalene + C_4-alkyl phenol isomers	T
225	C_3-alkyl phenol isomer	45
225	C_2-alkyl naphthalene isomer	T
227	ethylphenol isomer	135
227	dimethylnaphthalene isomer	T
228	C_2-alkyl phenol isomer	825
230	dimethylphenol isomer	T
230	ethylphenol isomer	T
231	cresol isomer	960
231	C_3-alkyl naphthalene isomer	T
232	C_2-alkyl naphthalene isomer	T
232		930
233	methylbiphenyl or $C_{13}H_{12}$ isomer	T
233	C_3-alkyl phenol isomer	T
235	ethylphenol isomer	T
236	C_3-alkyl phenol isomer	45
237	C_2-alkyl phenol isomer	72
239	C_3-alkyl phenol isomer	18
240	C_3-alkyl naphthalene isomer	T
240	acenaphthene	9
240	C_4-alkyl phenol isomer	T
240	C_3-alkyl phenol isomer	T
240	C_4-alkyl phenol isomer	T
240	C_3-alkyl naphthalene isomer	T
240	C_4-alkyl phenol isomer + biphenylene (tent.)	T
240	C_3-alkyl phenol isomer	T
240	C_4-alkyl phenol isomer	T
240	C_3-alkyl naphthalene isomer	T
240	C_4-alkyl phenol isomer	T
240	C_3-alkyl naphthalene isomer	T
240	C_4-alkyl phenol isomer	T
240	fluorene	T
240	anthracene or $C_{14}H_{10}$ isomer	T

Table D7. SEMI-VOLATILE ORGANICS IN TAR (-3T) FROM KNOCK-OUT CHAMBER DURING LOW BTU GASIFICATION OF ROSEBUD COAL (MERC, ERDA)

Elution Temperature (°C)	Compound	ppm
92	CO_2	NQ
97	acetone	NQ
99	C_4H_8O isomer	NQ
101	hydrocarbon (?)	T
101	$C_{10}H_{22}$ isomer	T
102	n-pentanal	NQ
105	n-decane	T
109	toluene	T
110	$C_{11}H_{24}$ isomer	T
113	n-undecane	T
117	$C_{11}H_{22}$ isomer	T
118	C_2-alkyl benzene isomer (tent.)	T
118	$C_{12}H_{26}$ isomer (tent.)	T
123	n-dodecane	530
128	C_3-alkyl benzene isomer	40
129	$C_{12}H_{24}$ isomer	160
131	C_3-alkyl benzene isomer	T
134	C_4-alkyl benzene isomer	T
135	n-tridecane	570
138	C_4-alkyl benzene isomer	T
139	n-butylbenzene + $C_{13}H_{26}$ isomer	T
141	$C_{13}H_{26}$ isomer	70
142	$C_{14}H_{30}$ isomer	T
143	trimethylbenzene isomer	10
144	$C_{14}H_{30}$ isomer	T
145	C_4-alkyl benzene isomer	T
146	C_4-alkyl benzene isomer	T
147	C_4-alkyl benzene isomer	T
148	n-tetradecane	460
148	n-nonanal	T
150	C_5-alkyl benzene isomer	T
151	methylindan + $C_{14}H_{28}$ isomers	T
152	C_5-alkyl benzene isomer	T
153	n-pentylbenzene	T
154	$C_{14}H_{28}$ isomer	T
156	C_5-alkyl benzene isomer	T
156	C_4-alkyl benzene isomer	T
157	C_5-alkyl benzene isomer	T
158	$C_{14}H_{28}$ isomer	T
161	n-pentadecane	T
162	n-decanal	T
163	indene	T
163	C_4-alkyl benzene isomer	T
164	$C_{11}H_{14}$ isomer	T
165	phenyl-n-hexane	T
167	$C_{11}H_{14}$ isomer	T
168	C_6-alkyl benzene isomer	T
170	hydrocarbon (?)	T
172	C_6-alkyl benzene isomer	T
173	C_3-alkyl indan isomer	T
174	n-hexadecane	T
176	methylindene isomer	190
177	$C_{12}H_{16}$ isomer	T
178	$C_{11}H_{14}$ isomer	T
178	methylindene isomer	T
180	trimethylindan isomer	T
181	C_7-alkyl benzene + $C_{11}H_{14}$ isomers	T
183	$C_{13}H_{18}$ isomer	T
185	$C_{11}H_{14}$ isomer	T
185	$C_{12}H_{16}$ isomer	T
186	$C_{17}H_{34}$ isomer	T
186	$C_{13}H_{18}$ isomer (tent.)	T
187	$C_{12}H_{16}$ isomer	T
188	dimethylbenzofuran isomer	T
188	$C_{13}H_{18}$ + $C_{11}H_{12}$ isomers	T
189	dimethylbenzofuran isomer	T
191	methyldihydronaphthalene isomer	T
192	phenyl-n-octane + $C_{17}H_{36}$ isomer	T
193	$C_{11}H_{12}$ isomer	T
193	C_8-alkyl benzene isomer	T
195	d_5-nitrobenzene (eS)	
196	naphthalene	2670
198	$C_{11}H_{12}$ isomer	T
199	trimethylindan isomer	T
200	$C_{13}H_{18}$ isomer (tent.)	T
201	$C_{14}H_{20}$ isomer	T
202	2,3-benzothiophene	T
204	$C_{13}H_{18}$ isomer	T
207	n-nonadecane	525
207	methylnaphthalene isomer	411
209	n-$C_{19}H_{40}$ isomer	T
212	methylnaphthalene isomer	230
214.	pentamethylindan isomer	150
217	$C_{19}H_{38}$ isomer	T
220	n-$C_{12}H_{42}$ isomer	T

(continued)

Table D7 (cont'd)

Elution Temperature (°C)	Compound	ppm	Elution Temperature (°C)	Compound	ppm
220	dimethylnaphthalene isomer	T			
222	phenol	T			
222	biphenyl	T			
223	dimethylnaphthalene isomer	T			
224	dimethylnaphthalene isomer	160			
225	$C_{12}H_{40}$ isomer	T			
228	dimethylphenol isomer	1490			
231	cresol isomer	T			
232	$\underline{n}$-$C_{21}H_{44}$ isomer	1710			
232	C_3-alkyl naphthalene isomer	10			
232	C_2-alkyl naphthalene isomer	13			
233	$C_{14}H_{40}$ isomer	12			
233	$C_{21}H_{42}$ isomer	10			
235	C_2-alkyl phenol isomer	17			
238	ethylphenol isomer	T			
239	acenaphthene	T			
239	C_3-alkyl phenol isomer	T			
240	C_2-alkyl phenol isomer	T			
240	ethylphenol isomer	T			
240	$\underline{n}$-$C_{22}H_{46}$ isomer (tent.)	T			
240	trimethylnaphthalene isomer	T			
240	biphenylene	T			
240	trimethylnaphthalene isomer	T			
240	dibenzofuran	T			
240	fluorene	T			
240	$C_{13}H_{10}O$ isomer (tent.)	T			
240	$C_{13}H_{10}O$ isomer (tent.)	T			
240	C_3-alkyl phenol isomer	T			
240	C_3-alkyl phenol isomer	T			
240	C_3-alkyl naphthalene isomer	T			

Table D8. SEMI-VOLATILE ORGANICS IN AQUEOUS CONDENSATE (-4L) DURING LOW BTU GASIFICATION OF ROSEBUD COAL (MERC, ERDA)

Elution Temperature (°C)	Compound	ppb
92	CO_2	NQ
95	acetaldehyde	NQ
97	ethyl formate	NQ
98	$C_{10}H_{22}$ isomer	T
99	*n*-nonane	3
99	ethyl acetate	NQ
99	aldehyde (?)	NQ
101	$C_{10}H_{22}$ isomer	27
103	dimethyl ether	NQ
103	$C_{11}H_{24}$ isomer	T
104	$C_{10}H_{22}$ isomer	T
104	$C_{12}H_{26}$ isomer	T
105	*n*-decane	129
105	$C_{13}H_{28}$ isomer	T
106	$C_{11}H_{24}$ isomer	T
108	$C_{10}H_{20}$ isomer	T
109	toluene	95
111	*n*-undecane	468
111	$C_6H_{12}O$ isomer	T
116	ethylbenzene	T
118	xylene isomer	63
119	$C_{13}H_{28}$ isomer	T
122	2-heptanone	48
123	*n*-dodecane	1420
124	cyclopentanone (tent.)	56
125	2-methylcyclopentanone	72
126	*n*-propylbenzene	T
128	ethyltoluene isomer	6
128	$C_7H_{12}O$ isomer	T
129	$C_{12}H_{24}$ isomer	51
131	$C_{12}H_{24}$ isomer	T
131	C_3-alkyl benzene isomer	T
135	octanone isomer	T
136	*n*-tridecane	2020
139	C_4-alkyl benzene isomer	T
143	C_4-alkyl benzene isomer	T
144	C_3-alkyl benzene isomer	96
146	C_4-alkyl benzene isomer	T
149	C_6H_8O isomer	T
149	indan + *n*-tetradecane	940
152	C_5-alkyl benzene isomer	760
153	$C_{10}H_{12}$ isomer	370
154	*n*-pentylbenzene	170
156	C_5-alkyl benzene isomer	T
156	$C_{14}H_{28}$ isomer	T
157	C_4-alkyl benzene + C_5-alkyl benzene isomers	17
158	$C_{15}H_{30}$ isomer	T
163	$C_{10}H_{12}$ isomer	T
164	*n*-pentadecane	110
165	indene	160
165	C_4-alkyl benzene isomer	T
166	$C_8H_{12}O$ + $C_{11}H_{14}$ + C_6-alkyl benzene isomers	T
167	benzofuran	880
167	methylindan isomer	84
168	phenyl-*n*-hexane	36
169	$C_{11}H_{14}$ isomer	T
170	dimethylindan isomer	54
171	C_6-alkyl benzene isomer	12
171	$C_{15}H_{30}$ isomer	T
172	$C_7H_{10}O$ isomer	110
174	$C_8H_{12}O$ isomer	24
175	C_5-alkyl benzene isomer	T
176	$C_{11}H_{14}$ isomer	T
176	$C_{17}H_{16}$ isomer	T
177	*n*-hexadecane (tent.)	T
178	methylindene isomer	T
179	methylbenzofuran isomer	28
180	cyanobenzene + dimethylindan isomer	23
180	methylindene isomer	96
181	phenyl-*n*-heptane	T
182	$C_{12}H_{16}$ isomer	T
183	$C_{11}H_{14}$ + C_7-alkyl benzene isomers	T
183	acetophenone	T
185	$C_{12}H_{16}$ isomer	T
186	$C_{13}H_{18}$ isomer	T
187	$C_{12}H_{16}$ isomer	T
187	$C_{13}H_{18}$ isomer	T
188	dimethylbenzofuran isomer	T
189	$C_{12}H_{16}$ isomer	T
190	methyldihydronaphthalene isomer	T
190	$C_{13}H_{18}$ isomer	T
191	dimethylbenzofuran isomer	T
192	alkylindan isomer	100
193	$C_{11}H_{12}$ isomer	36
194	phenyl-*n*-octane	T

(continued)

Table D8 (cont'd)

Elution Temperature (°C)	Compound	ppb
195	$C_{11}H_{12}$ isomer	84
196	C_8-alkyl benzene isomer	T
196	d_5-nitrobenzene (es)	
197	naphthalene	5700
210	methylnaphthalene isomer	2510
212	$C_{13}H_{18}$ isomer	66
213	$C_{12}H_{14}$ isomer	T
214	dimethylphenol + methylnaphthalene isomers	2440
215	$C_{13}H_{18}$ isomer	T
216	$C_{14}H_{20}$ isomer	T
217	$C_{13}H_{12}$ isomer (tent.)	T
218	pentamethylindan or tetramethylindanone isomer	100
220	C_3-alkyl phenol isomer	42
221	ethylnaphthalene isomer	30
223	dimethylnaphthalene isomer	110
223	cresol isomer	4830
224	phenol	280
224	C_3-alkyl phenol isomer	T
225	biphenyl	160
227	C_2-alkyl naphthalene isomer	530
229	C_3-alkyl phenol isomer	84
230	ethylnaphthalene isomer	T
230	dimethylnaphthalene isomer	T
231	ethylphenol isomer	1360
232	dimethylphenol isomer	4990
232	C_4-alkyl phenol isomer	110
232	cresol + C_3-alkyl naphthalene isomers	42
234	C_2-alkyl naphthalene isomer	T
234	cresol isomer	4490
236	$C_{13}H_{12}$ isomer	T
237	C_3-alkyl naphthalene isomer	T
237	C_3-alkyl phenol isomer	36
238	dimethylnaphthalene isomer	T
238	C_3-alkyl phenol isomer	90
239	C_2-alkyl phenol isomer	30
240	C_3-alkyl phenol isomer	21
240	C_2-alkyl phenol + C_3-alkyl naphthalene isomers	12
240	ethylphenol + acenaphthene	110
240	C_4-alkyl phenol + C_2-alkyl naphthalene isomers	T
240	C_4-alkyl phenol isomer	T
240	C_2-alkyl naphthalene isomer	T
240	C_3-alkyl phenol isomer	T
240	C_2-alkyl naphthalene isomer	280
240	dibenzofuran	72
240	fluorene	24
240	unknown	NQ

Table D9. SEMI-VOLATILE ORGANICS IN TAR (-5T) FROM KNOCK-OUT CHAMBER DURING LOW BTU GASIFICATION OF ROSEBUD COAL (MERC, ERDA)

Elution Temperature (°C)	Compound	ppm
92	CO_2	NQ
97	acetone	NQ
98	hydrocarbon (?)	T
114	n-dodecane	T
124	n-tridecane	240
162	C_3-alkyl indan isomer + n-pentylbenzene	T
195	d_5-nitrobenzene (eI)	
196	naphthalene	1300
209	methylnaphthalene isomer	350
213	methylnaphthalene isomer	100
216	pentamethylindan isomer	T
219	C_2-alkyl naphthalene isomer	T
221	n-$C_{20}H_{42}$ isomer	11000
221	dimethylnaphthalene isomer	T
222	phenol	400
224	biphenyl	T
225	dimethylnaphthalene isomer	T
226	dimethylnaphthalene isomer	700
229	dimethylphenol isomer	25000
231	cresol isomer	17600
232	n-$C_{21}H_{44}$ isomer	T
234	$C_{14}H_{10}$ isomer	T
237	C_2-alkyl phenol isomer	130
238	C_2-alkyl phenol + $C_{14}H_{10}$ isomers	150
239	C_3-alkyl naphthalene isomer	T
240	ethylphenol isomer	170
240	acenaphthene	180
240	n-$C_{22}H_{46}$ (tent.)	T

Table D10. SEMI-VOLATILE ORGANICS IN AQUEOUS CONDENSATE (-6L) FROM LOW BTU GASIFICATION OF ROSEBUD COAL (MERC, ERDA)

Elution Temperature (°C)	Compound	ppb	Elution Temperature (°C)	Compound	ppb
92	CO_2	NQ	232	dimethylphenol isomer	28800
95	acetaldehyde	NQ	233	cresol isomer	29500
97	acetone	NQ	237	C_3-alkyl phenol isomer	T
97	ethyl formate	1200	238	C_3-alkyl phenol isomer	T
99	ethyl acetate	NQ	239	dimethylphenol isomer	T
101	dimethyl ether	NQ	240	C_3-alkyl phenol isomer	T
102	$C_{10}H_{22}$ isomer	T	240	C_2-alkyl phenol isomer	11000
104	hydrocarbon (?)	T	240	C_2-alkyl phenol isomer	10800
196	d_5-nitrobenzene (es)		240	C_3-alkyl phenol isomer	T
200	naphthalene	1500	240	C_3-alkyl phenol isomer	1000
223	cresol isomer	35000	240	C_3-alkyl phenol + C_3-alkyl naphthalene isomers	200
224	phenol	41000			
231	ethylphenol isomer	5000	240	C_3-alkyl phenol isomer	160

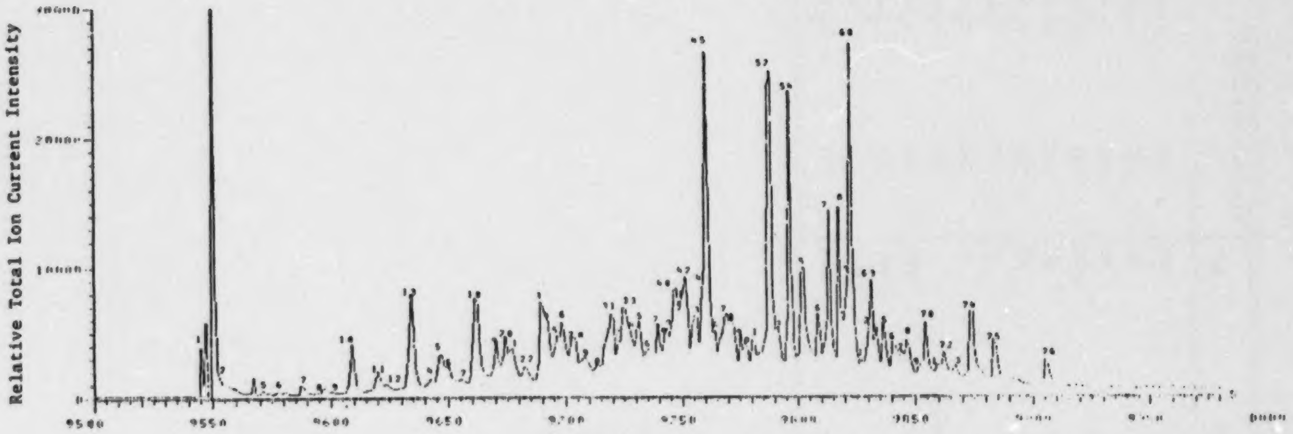


Figure D6. Profile of semi-volatile organics in neutral fraction of tar condensate (-7T) from low btu Rosebud coal gasification (MERC, ERDA).

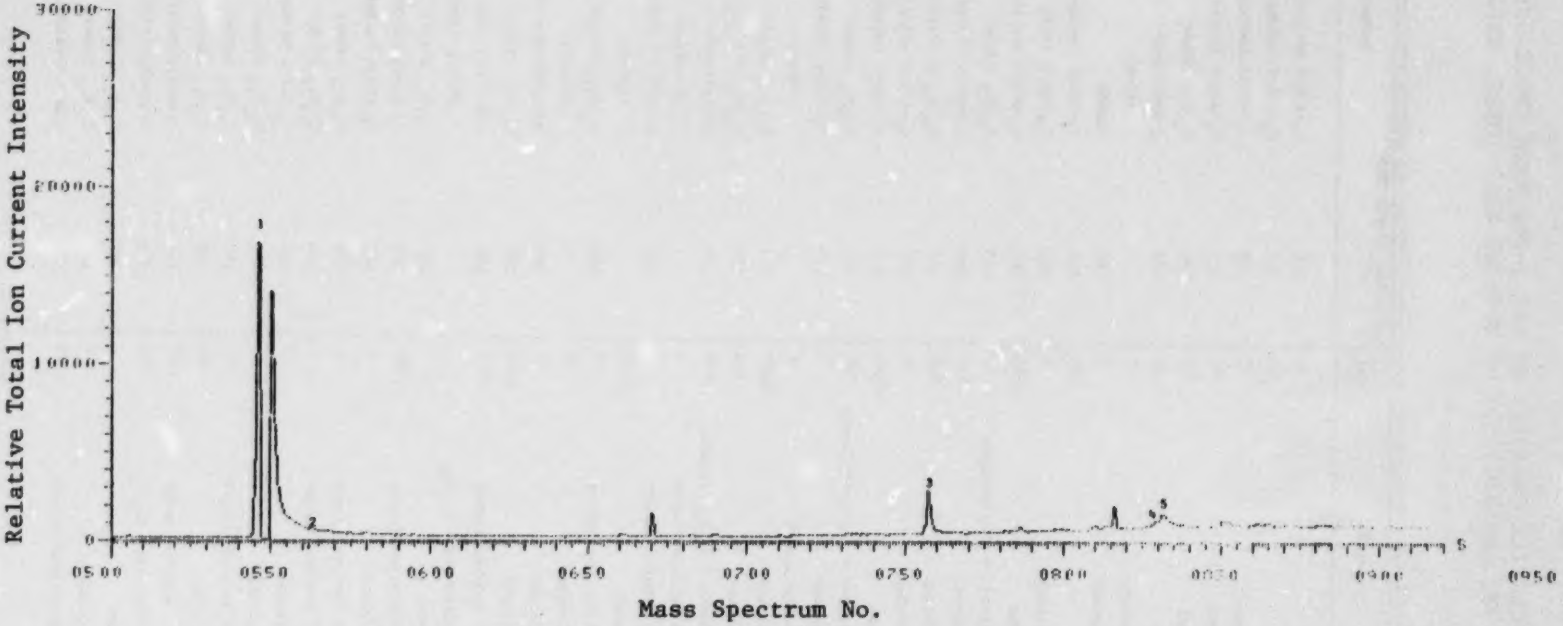


Figure D7 . Profile of semi-volatile organics in basic fraction of tar-condensate (-7T) from low btu gasification of Rosebud coal (MERC, ERDA).

Table D11. SEMI-VOLATILE ORGANICS IN TAR (-7T) FROM KNOCK-OUT CHAMBER DURING LOW BTU GASIFICATION OF ROSEBUD COAL (MERC, ERDA)

Elution Temperature (°C)	Compound	ppm
92	CO_2	NQ
97	acetone	NQ
101	C_4H_8O isomer	T
101	hydrocarbon (?)	NQ
104	n-pentanal	NQ
105	n-decane	20
107	$C_{10}H_{20}$ isomer	T
108	$C_{11}H_{24}$ isomer	T
109	toluene	465
110	$C_{11}H_{24}$ isomer	T
113	n-undecane	1650
117	$C_{11}H_{22}$ isomer + ethylbenzene	T
118	$C_{11}H_{22}$ isomer	230
119	$C_{12}H_{24}$ isomer	210
122	$C_{12}H_{24}$ isomer	T
124	n-dodecane	6560
127	$C_8H_{14}O$ isomer + n-propylbenzene	760
127	$C_{12}H_{24}$ isomer	T
128	ethyltoluene isomer	T
129	$C_{12}H_{24}$ isomer	2100
130	$C_{13}H_{28}$ isomer	410
131	ethyltoluene + $C_{12}H_{24}$ isomers	120
133	C_3-alkyl benzene isomer	T
134	C_4-alkyl benzene isomer	T
136	n-tridecane	12100
138	C_4-alkyl benzene isomer	T
140	n-butylbenzene	50
141	$C_{13}H_{26}$ isomer	T
142	$C_{13}H_{26}$ isomer	2050
143	C_4-alkyl benzene isomer	2270
144	trimethylbenzene + $C_{14}H_{28}$ isomers	
145	C_4-alkyl benzene isomer	1880
146	$C_{13}H_{26}$ isomer	T
146	C_4-alkyl benzene isomer	T
147	C_4-alkyl benzene isomer	T
148	$C_{14}H_{28}$ isomer	20
149	n-tetradecane	12270
152	C_5-alkyl benzene isomer	110
152	$C_{10}H_{12}$ isomer	90
153	C_5-alkyl benzene isomer	3080
154	n-pentylbenzene + $C_{14}H_{28}$ isomer	590
154	$C_{15}H_{30}$ isomer	T
155	C_5-alkyl benzene isomer	210
156	C_5-alkyl benzene isomer	2050
157	C_4-alkyl benzene isomer	410
158	C_5-alkyl benzene isomer	1960
159	C_6-alkyl benzene isomer	460
160	$C_{15}H_{30}$ isomer	T
163	n-pentadecane + methylindan isomer	3590
164	indene	7100
165	C_4-alkyl benzene isomer	550
166	C_2-alkyl indan isomer	T
166	C_6-alkyl benzene isomer	320
167	$C_{10}H_{12}$ isomer	380
168	phenyl-n-hexane	3150
169	$C_{15}H_{30}$ + dimethylindan isomers	760
170	C_6-alkyl benzene isomer	2310
172	C_7-alkyl benzene isomer	630
173	$C_{15}H_{30}$ isomer	550
175	C_5-alkyl benzene + $C_{11}H_{14}$ isomers	140
176	$C_{12}H_{16}$ isomer	T
176	$C_{16}H_{34}$ + $C_{11}H_{14}$ isomers	T
178	methylindene isomer + n-hexadecane	4250
179	C_7-alkyl benzene + $C_{12}H_{16}$ isomers	160
180	$C_{11}H_{12}$ (tent.) + alkyl indan isomers	470
180	methylindene isomer	8250
181	$C_{16}H_{32}$ isomer	2310
181	trimethylindan isomer + phenyl-n-heptane	730
183	$C_{11}H_{14}$ isomer	T
183	C_7-alkyl benzene isomer	325
185	C_8-alkyl benzene isomer	150
185	$C_{12}H_{16}$ isomer	T
186	$C_{13}H_{18}$ isomer	T
186	C_8-alkyl benzene isomer	T
187	$C_{13}H_{18}$ isomer	2190
187	$C_{11}H_{14}$ isomer	420
188	$C_{12}H_{16}$ isomer	T
189	dimethylbenzofuran isomer	T
190	trimethylindan isomer	1570
190	$C_{11}H_{12}$ isomer	T
191	$C_{13}H_{18}$ isomer	5130
192	dimethylbenzofuran isomer	7770

(continued)

Table D11 (cont'd)

Elution Temperature (°C)	Compound	ppm
193	$C_{13}H_{18}$ isomer	1710
194	$C_{11}H_{12}$ isomer	T
195	phenyl-*n*-octane	230
196	methyldihydronaphthalene isomer	2810
197	C_8-alkyl benzene isomer	5100
197	d_5-nitrobenzene (e#)	
198	naphthalene	21350
199	*n*-octadecane	T
201	$C_{11}H_{12}$ isomer	480
202	$C_{12}H_{16}$ isomer	2410
203	C_9-alkyl benzene + alkyl indan (tent.) isomers	2370
205	2,3-benzothiophene	1880
206	$C_{12}H_{16}$ or $C_{11}H_{12}O$ isomer	1410
206	$C_{14}H_{20}$ isomer	T
207	tetramethylindan or $C_{13}H_{18}$ isomers + phenyl-*n*-nonane	1550
208	$C_{13}H_{18}$ isomer	T
211	methylnaphthalene isomer	16410
211	*n*-nonadecane	12110
212	$C_{14}H_{20}$ isomer	370
213	methylquinoline (tent.) + alkyl indan isomers	210
215	methylnaphthalene isomer	17200
218	pentamethylindan isomer	6270
221	ethylnaphthalene isomer	4030
223	dimethylnaphthalene isomer	8150
225	biphenyl	8210
227	dimethylnaphthalene isomer	1760
228	dimethylnaphthalene isomer	18230
231	ethylnaphthalene isomer	710
232	dimethylphenol isomer	2760
232	dimethylnaphthalene + cresol isomers	2100
233	C_3-alkyl naphthalene isomer	550
234	*n*-$C_{20}H_{42}$ isomer	510
235	C_2-alkyl naphthalene isomer	3870
237	methylbiphenyl isomer	410
238	isopropylnaphthalene isomer	1780
239	trimethylnaphthalene isomer	470
240	C_3-alkyl naphthalene isomer	T
240	C_4-alkyl naphthalene isomer	430
240	C_3-alkyl naphthalene isomer	T
240	C_2-alkyl phenol isomer	2190
240	acenaphthene	4380
isothermal	C_3-alkyl naphthalene isomer	T
	C_3-alkyl naphthalene isomer	140
	C_3-alkyl naphthalene isomer	1210
	C_4-alkyl naphthalene isomer	T
	biphenylene	290
	C_5-alkyl naphthalene isomer	T
	C_3-alkyl naphthalene isomer	7810
	$C_{21}H_{42}$ isomer	T
	dibenzofuran	4030
	$C_{14}H_{12}$ isomer (tent.)	T
	fluorene	470
	$C_{13}H_{10}O$ isomer (tent.)	1890

Table D12. SEMI-VOLATILE ORGANICS IN WATER (-1L) FROM DEWATERING WELL #5 PRIOR TO *IN SITU* COAL GASIFICATION (LLL, ERDA)

Elution Temperature (°C)	Compound	ppb	Elution Temperature (°C)	Compound	ppb
92	CO_2	NQ	197	d_5-nitrobenzene (eS)	
97	acetone	NQ	225	phenol	15
98	ethyl formate	33	227	ethylphenol isomer	6
99	*n*-butanal (tent.)	T	232	dimethylphenol isomer	360
100	ethyl acetate	300	234	cresol isomer	132
101	hydrocarbon (?)	NQ	235	C_2-alkyl phenol isomer	T
103	benzene	T	237	C_3-alkyl phenol isomer	T
104	*n*-decane	T	239	dimethylphenol isomer	T
105	$C_5H_{10}O$ isomer	6	240	C_3-alkyl phenol isomer	T
110	toluene	6	240	C_2-alkyl phenol isomer	T
112	*n*-hexanal	120	240	ethylphenol isomer	T

Table D13. SEMI-VOLATILE ORGANICS IN LIQUID BLEND FROM DEWATERING WELLS #1 and 6 PRIOR TO IN SITU COAL GASIFICATION (LLL, ERDA)

Elution Temperature (°C)	Compound	ppb	Elution Temperature (°C)	Compound	ppb
93	CO_2	NQ	197	d_5-nitrobenzene (eI)	
96	acetaldehyde	NQ	224	cresol isomer	189
98	acetone	NQ	225	phenol + C_3-alkyl phenol isomer	27
98	ethyl formate	60	231	ethylphenol isomer	T
100	hydrocarbon (?)	NQ	234	dimethylphenol isomer	T
100	ethyl acetate	630	235	cresol isomer	19.8
101	dimethyl ether	90	235	C_3-alkyl phenol isomer	T
101	methyl ethyl ketone (tent.)	T	238	C_3-alkyl phenol isomer	T
102	n-nonane	T	240	dimethylphenol isomer	T
103	$C_{10}H_{22}$ isomer	T	240	C_3-alkyl phenol isomer	T
104	hydrocarbon (?)	NQ	240	dimethylphenol isomer	T
105	n-pentanal	T	240	ethylphenol isomer	T
109	toluene	117	240	acenaphthene (tent.)	T
111	n-hexanal	T	240	C_4-alkyl phenol isomer	T
158	aldehyde isomer (?)	NQ	240	C_3-alkyl phenol isomer	T
159	acetic acid	T	240	C_3-alkyl phenol isomer	T
169	benzaldehyde	T			

Table D14. SEMI-VOLATILE ORGANICS IN PROCESS WATER (-3L) DURING IN SITU COAL GASIFICATION (LLL, ERDA)

Elution Temperature (°C)	Compound	ppm
92	CO_2	NQ
94	diethyl ether	NQ
95	acetaldehyde	NQ
97	ethyl formate	NQ
100	ethyl acetate	NQ
101	methyl ethyl ketone	T
103	methyl isopropyl ketone	T
105	2-pentanone	10
109	toluene	50
111	dimethyl disulphide	50
123	unknown	NQ
125	cyclopentanone	110
126	2-methylcyclopentanone	20
128	3-methylcyclopentanone	14
130	methylpyridine isomer	4
142	dimethylcyclopentanone isomer	T
143	$C_7H_{10}O$ (ketone?)	T
144	anisole	T
145	$C_7H_{10}O$ (ketone?)	T
147	C_6H_7O (ketone?)	NQ
157	p-methylanisole	22
168	$C_8H_{12}O$ isomer	5
168	n-nonanoic acid	5
172	C_6H_8O isomer	7
175	$C_7H_{10}O$ or C_8H_{16} isomer	150
177	$C_8H_{12}O$ isomer	20
178	benzonitrile	40
179	$C_8H_{12}O$ isomer	T
180	n-decanoic acid	3
181	phenyl acetate	4
193	n-undecanoic acid	5
194	cresyl acetate (?)	T
196	cresyl acetate (?)	T
196	d_5-nitrobenzene (es)	146
197	naphthalene	26
212	dimethylphenol isomer	T
213	methylnaphthalene isomer	T
214	C_3-alkyl phenol isomer (tent.)	T
217	C_3-alkyl phenol isomer	T
219	cresol isomer + phenol	50000
222	C_3-alkyl phenol isomer	4000
226	$C_{10}H_{14}O$ isomer	10
228	ethylphenol isomer	6000
229	dimethylphenol + cresol isomers	48000
236	C_3-alkyl phenol isomer	400
237	dimethylphenol isomer	425
239	ethylphenol isomer	455
240	C_3-alkyl phenol isomer	600
240	dimethylphenol isomer	3800
240	ethylphenol isomer	400
240	C_3-alkyl phenol isomer	350
240	C_2-alkyl phenol isomer	1600
240	C_3-alkyl phenol isomer	20
240	C_3-alkyl phenol isomer	25
240	C_3-alkyl phenol isomer	T
240	$C_{10}H_{10}O$ isomer	T
240	aldehyde (?)	NQ
240	C_2-alkyl benzaldehyde isomer	850
240	C_2-alkyl benzaldehyde	450

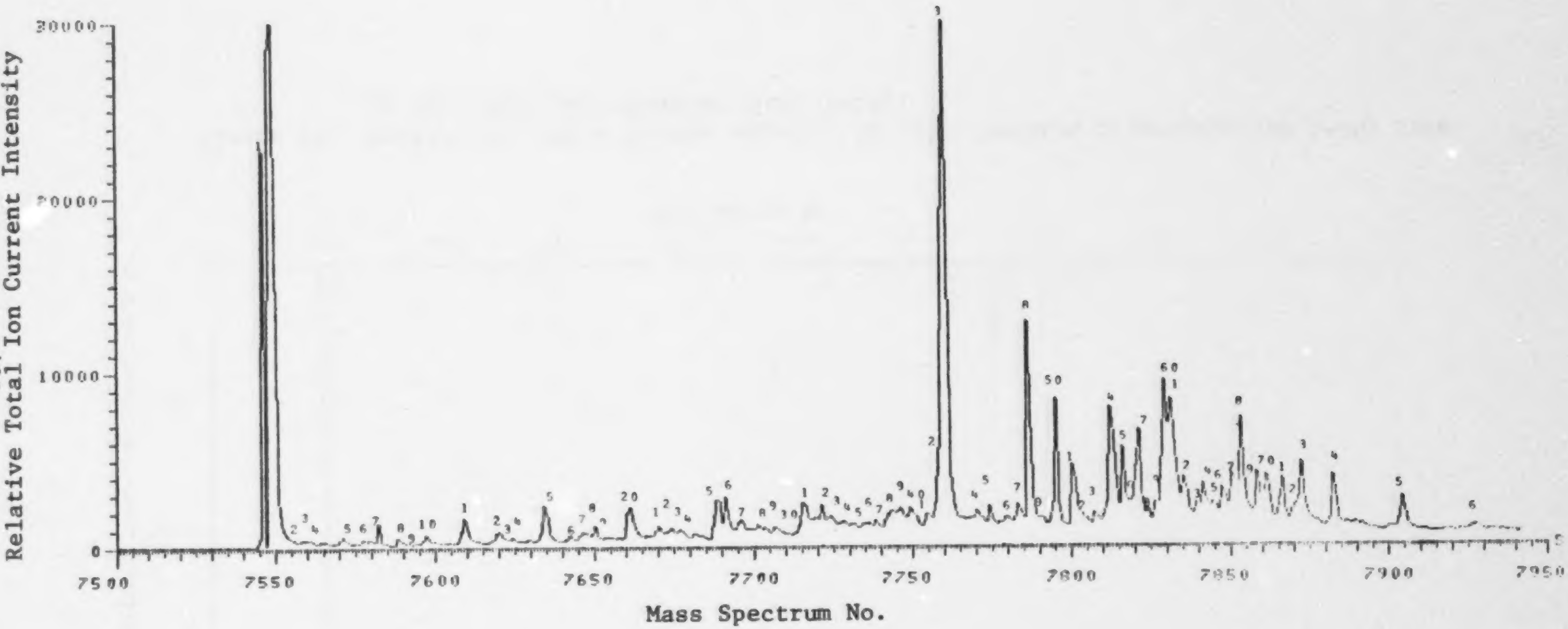


Figure D8. Profile of semi-volatile organics in neutral fraction of process tar (-4L) from in situ coal gasification (LLL, ERDA).

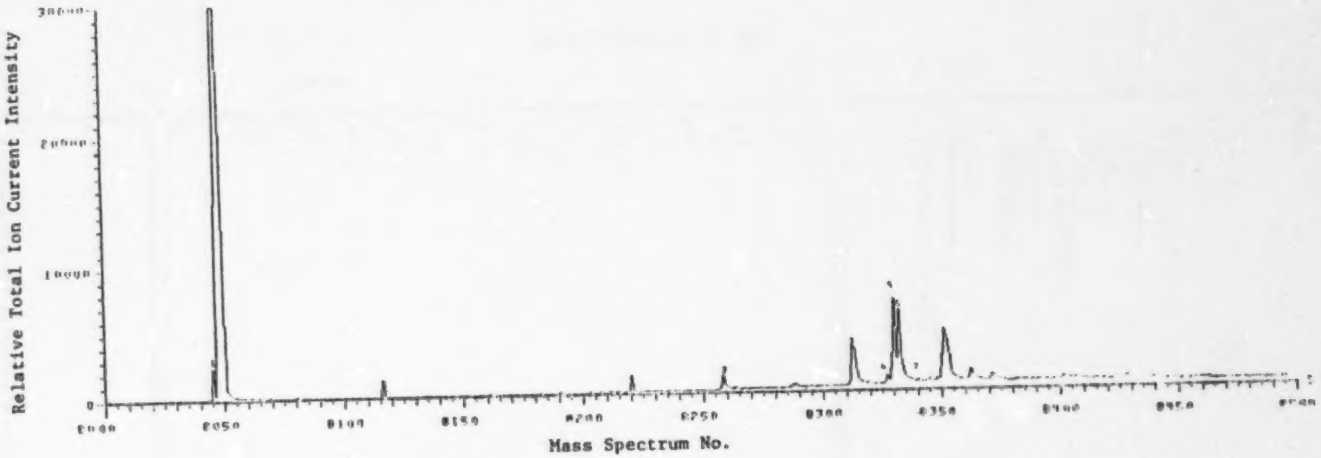


Figure D9. Profile of semi-volatile organics in acid fraction of process tar (-4L) from *in situ* coal gasification (LLL, ERDA).

Table D15. SEMI-VOLATILE ORGANICS IN PROCESS TAR (-4T) FROM *IN SITU* COAL GASIFICATION (LLL, ERDA)

Elution Temperature (°C)	Compound	ppm
92	CO_2	NQ
97	acetone	NQ
102	hydrocarbon (?)	NQ
110	$C_{11}H_{24}$ isomer	T
113	*n*-undecane	140
116	ethylbenzene	26
117	$C_{11}H_{22}$ isomer	T
118	xylene isomer	124
122	$C_7H_{14}O$ isomer	42
123	xylene isomer	T
123	*n*-$C_{12}H_{26}$ isomer	1240
127	*n*-propylbenzene	420
127	ethyltoluene isomer	420
128	$C_{12}H_{24}$ isomer	T
128	C_3-alkyl benzene isomer	T
129	$C_{12}H_{24}$ isomer	570
131	$C_{13}H_{26}$ + trimethylbenzene isomers	33
134	C_3-alkyl benzene isomer	57
135	C_4-alkyl benzene isomer	T
137	*n*-tridecane + trimethylbenzene isomers	2730
140	C_4-alkyl benzene isomer	930
140	$C_{13}H_{26}$ isomer	660
141	*n*-butylbenzene	72
143	$C_{13}H_{26}$ isomer	420
144	trimethylbenzene isomer	540
146	C_4-alkyl benzene isomer	T
147	C_4-alkyl benzene isomer	T
149	*n*-tetradecane + indan	2790
152	C_5-alkyl benzene isomer	1410
152	methylinden isomer	420
153	C_5-alkyl benzene isomer	T
154	*n*-pentylbenzene	270
156	$C_{14}H_{28}$ isomer	45
157	C_5-alkyl benzene isomer	T
157	C_4-alkyl benzene + $C_{14}H_{28}$ isomers	51
158	C_5-alkyl benzene + $C_{14}H_{28}$ isomers (tent.)	T
159	C_6-alkyl benzene isomer (tent.)	30
163	*n*-pentadecane	2790
164	indene	1440
165	C_4-alkyl benzene isomer	T
166	C_2-alkyl indan isomer	T
167	methylindan isomer	510
167	phenyl-*n*-hexane	60
168	$C_{15}H_{30}$ isomer	T
169	C_2-alkyl indan + $C_{15}H_{30}$ isomers	93
170	C_6-alkyl benzene isomer	54
171	$C_7H_{10}O$ isomer	171
174	C_6-alkyl benzene isomer	T
175	$C_{11}H_{14}$ isomer	T
175	$C_{12}H_{16}$ isomer	T
176	*n*-$C_{16}H_{34}$ isomer	2190
177	methylindene isomer	450
178	alkyl indan isomer	660
180	methylindene isomer	270
181	C_3-alkyl indan isomer	T
182	$C_{16}H_{32}$ isomer	T
183	C_7-alkyl benzene + C_2-alkyl indan isomers	26
183	$C_{16}H_{32}$ isomer	T
184	alkyl benzene isomer	45
185	C_4-alkyl indan isomer	T
186	$C_{11}H_{14}$ isomer	81
186	$C_{12}H_{16}$ isomer	T
187	$C_{18}H_{36}$ isomer	T
188	*n*-heptadecane	87
191	$C_{13}H_{18}$ isomer	T
192	dimethylbenzofuran isomer (tent.)	42
193	$C_{11}H_{12}$ isomer	T
194	phenyl-*n*-octane	33
195	$C_{17}H_{34}$ isomer	T
195	methyldihydronaphthalene isomer	T
197	d_5-nitrobenzene (eS)	
198	naphthalene	17930
199	$C_{13}H_{18}$ isomer	270
200	$C_{14}H_{20}$ isomer	T
201	$C_{11}H_{12}$ isomer	T
202	$C_{12}H_{16}$ isomer	T
203	trimethylindan isomer	130
203	$C_{13}H_{18}$ isomer	T
205	2,3-benzothiophene	190
207	phenyl-*n*-nonane	40
208	$C_{15}H_{22}$ isomer (tent.)	T
208	$C_{18}H_{38}$ isomer	T
209	$C_{14}H_{20}$ isomer (tent.)	260
211	methylnaphthalene isomer	611

(continued)

Table D15 (cont'd)

Elution Temperature (°C)	Compound	ppm
212	$C_{19}H_{40}$ isomer	170
212	alkyl indan isomer	23
213	$C_{19}H_{38}$ isomer	27
214	dimethylphenol isomer	T
215	methylnaphthalene isomer	4110
217	pentamethylindan isomer	1930
219	$C_{15}H_{22}$ + C_3-alkyl phenol isomers	370
220	$C_{19}H_{38}$ isomer	T
220	phenyl-*n*-decane	T
221	ethylnaphthalene isomer	130
222	$C_{15}H_{20}$ isomer	T
223	phenol + cresol + dimethylnaphthalene isomers	3860
223	*n*-$C_{20}H_{42}$ isomer	490
226	biphenyl	1390
227	dimethylnaphthalene isomer	T
228	dimethylnaphthalene isomer	2150
229	C_3-alkyl phenol isomer	110
230	ethylphenol isomer	180
231	dimethylphenol isomer	T
232	cresol isomer	4050
233	cresol isomer	3870
234	C_2-alkyl naphthalene + C_3-alkyl naphthalene isomers	660
236	methylbiphenyl isomer	13
237	C_4-alkyl naphthalene isomer	27
237	C_3-alkyl phenol isomer	410
238	C_3-alkyl naphthalene isomer	T
238	C_3-alkyl phenol isomer	37
239	C_2-alkyl phenol isomer	T
239	C_3-alkyl naphthalene isomer	T
240	C_3-alkyl phenol isomer	620
240	ethylphenol isomer	850
240	acenaphthene	2560
240	C_4-alkyl phenol isomer	410
240	C_4-alkyl naphthalene isomer	T
240	C_3-alkyl naphthalene isomer	1380
240	C_3-alkyl phenol isomer	1360
240	C_4-alkyl phenol isomer	T
240	biphenylene	1460
240	C_3-alkyl phenol isomer	T
240	C_5-alkyl naphthalene isomer	T
240	C_3-alkyl naphthalene isomer	1560
240	C_4-alkyl phenol isomer	T
240	dibenzofuran	1480
240	C_4-alkyl phenol isomer	T
240	fluorene	990
240	hydroxyfluorene or $C_{13}H_{10}O$ isomer	T

Table D16. SEMI-VOLATILE ORGANICS IN WATER (-5L) FROM PERMEATION WELL #5 (LLL, ERDA)

Elution Temperature (°C)	Compound	ppb	Elution Temperature (°C)	Compound	ppb
94	CO_2	NQ	165	n-decanal (tent.)	6.6
97	acetaldehyde	NQ	168	unknown	NQ
99	ethyl formate	720	169	aldehyde (?)	NQ
100	acetone	NQ	184	acetic acid (tent.)	T
101	ethyl acetate	810	191	alcohol (?)	NQ
103	dimethyl ether (tent.)	135	202	d_5-nitrobenzene (es)	
105	hydrocarbon (?)	NQ	230	phenol	72
107	n-butanal	3	238	dimethylphenol isomer	186
109	hydrocarbon (tent.)	NQ	239	cresol isomer	364
112	toluene	T	240	ethylphenol isomer	9
114	n-hexanal (tent.)	T	240	C_2-alkyl phenol isomer	69
141	n-octanal	3	240	C_2-alkyl phenol isomer	72
144	unknown	NQ	240	C_3-alkyl phenol isomer	T
146	hydrocarbon (tent.)	T	240	C_2-alkyl phenol isomer	T
155	n-nonanal	34	240	C_3-alkyl phenol isomer	9
162	acetoxy acetone (?)	NQ	240	ethylphenol isomer	33

Table D17. SEMI-VOLATILE ORGANICS IN PROCESS COMPOSITE (-6L) FROM *IN SITU* COAL GASIFICATION (LLL, ERDA)

Elution Temperature (°C)	Compound	ppm
92	CO_2	NQ
94	diethyl ether	NQ
97	ethyl formate	NQ
100	*n*-nonane	520
100	ethyl acetate	NQ
101	dimethyl ether	NQ
102	$C_{10}H_{22}$ isomer	15
102	hydrocarbon (?)	NQ
103	$C_5H_{10}O$ isomer	10
104	C_9H_{18} isomer	T
104	$C_{10}H_{2}\,O$ isomer	T
105	*n*-decane	580
106	$C_{10}H_{20}$ isomer	210
107	toluene	30
107	C_9H_{18} isomer (tent.)	T
108	$C_{10}H_{20}$ isomer	550
110	$C_{11}H_{22}$ isomer	T
110	$C_{11}H_{24}$ isomer	45
111	$C_6H_{12}O$ isomer	170
112	$C_{11}H_{24}$ isomer	T
112	$C_{10}H_{20}$ isomer	62
113	$C_{11}H_{22}$ isomer	49
114	*n*-undecane	550
116	ethylbenzene	1210
117	$C_{11}H_{22}$ isomer	5620
117	xylene isomer	380
118	$C_{11}H_{22}$ isomer	460
119	$C_{12}H_{26}$ isomer	T
120	$C_{11}H_{22}$ isomer	47
121	$C_7H_{14}O$ isomer	T
121	$C_{12}H_{26}$ isomer	91
122	xylene isomer	760
122	$C_{11}H_{22}$ isomer	28
123	$C_{13}H_{28}$ isomer	T
124	$C_{12}H_{26}$ isomer	7
124	*n*-dodecane	2050
125	*n*-propyl benzene	T
125	$C_{12}H_{24}$ isomer	79
127	ethyltoluene isomer	3820
128	$C_{12}H_{24}$ isomer	T
129	trimethylbenzene + $C_{12}H_{24}$ isomers	3850
129	$C_{12}H_{24}$ isomer	T
130	C_3-alkyl benzene isomer	T
131	C_3-alkyl benzene + $C_{13}H_{26}$ isomers	460
132	$C_{12}H_{24}$ isomer	T
132	$C_{13}H_{28}$ isomer	T
132	methylpyridine isomer	20000
133	$C_8H_{16}O$ isomer	5260
134	trimethylbenzene isomer	550
134	C_3-alkyl benzene isomer	T
134	dimethylpyridine isomer	310
135	$C_{13}H_{28}$ isomer	460
135	C_4-alkyl benzene + $C_{13}H_{26}$ isomers	NQ
136	$C_{13}H_{26}$ isomer	110
137	$C_{13}H_{28}$ isomer	T
137	*n*-tridecane + C_4-alkyl benzene isomer	320
138	*n*-butylbenzene + $C_{13}H_{26}$ isomer	2050
138	C_3-alkyl benzene isomer	T
138	ethylpyridine isomer	4250
139	$C_{13}H_{28}$ isomer	540
139	$C_8H_{11}N$ isomer	660
140	C_4-alkyl benzene + $C_{13}H_{26}$ isomers	T
140	C_4-alkyl benzene + $C_{14}H_{28}$ isomers	T
141	trimethylbenzene isomer	8050
141	*n*-butylbenzene	32
141	dimethylpyridine isomer	T
142	$C_{14}H_{30}$ isomer (tent.)	56
142	$C_{14}H_{28}$ isomer	49
143	$C_{13}H_{26}$ isomer	570
143	C_4-alkyl benzene isomer	T
143	$C_8H_{11}N$ isomer	T
144	$C_{15}H_{32}$ isomer	T
144	C_4-alkyl benzene + $C_{14}H_{28}$ isomers	271
144	$C_9H_{13}N$ isomer	T
145	C_4-alkyl benzene isomer	T
145	unknown + $C_{13}H_{26}$ isomer	321
146	C_6H_8O + $C_{14}H_{30}$ isomers	T
146	$C_8H_{11}N$ isomer	T
146	indan	6550
147	$C_9H_{18}O$ isomer	1310
147	C_4-alkyl benzene + hydrocarbon (?)	T

(continued)

Table D17 (cont'd)

Elution Temperature (°C)	Compound	ppm
147	dimethylpyridine isomer	4200
148	C_4-alkyl benzene isomer	T
148	C_3-alkyl pyridine isomer	8140
149	C_7-alkyl cyclohexane + C_5-alkyl benzene isomers	T
149	dimethylpyridine isomer	6310
150	$C_{10}H_{12}$ isomer	T
150	n-tetradecane	2050
150	$C_{14}H_{30}$ isomer	T
150	C_3-alkyl pyridine isomer	220
152	n-pentylbenzene	1470
152	$C_{10}H_{12}$ isomer	T
154	C_5-alkyl benzene isomer	1860
154	$C_{14}H_{28}$ + $C_{15}H_{30}$ isomers	1430
155	C_4-alkyl benzene isomer	1310
155	$C_{14}H_{30}$ isomer	NQ
156	$C_{16}H_{34}$ isomer	1930
156	C_5-alkyl benzene isomer	T
158	$C_{14}H_{28}$ isomer	5100
158	C_4-alkyl benzene + $C_{14}H_{28}$ isomers	570
159	$C_{15}H_{30}$ isomer	1910
160	C_7-alkyl benzene isomer (tent.)	580
160	C_6-alkyl benzene isomer	T
161	$C_{15}H_{32}$ isomer	T
161	$C_{16}H_{34}$ isomer	T
163	C_4-alkyl benzene isomer	1470
163	benzofuran	9150
163	$C_{11}H_{14}$ isomer	3200
163	$C_{10}H_{12}$ isomer	1460
164	C_4-alkyl benzene + $C_{15}H_{32}$ isomers	1760
165	n-pentadecane	2810
165	C_6-alkyl benzene isomer	470
166	benzaldehyde	6550
166	$C_{11}H_{14}$ isomer	270
166	$C_{10}H_{12}$ isomer	14
167	$C_{11}H_{14}$ + $C_{15}H_{32}$ isomers	T
168	$C_{15}H_{30}$ isomer	T
168	phenyl-n-hexane	T
169	n-pentadecane	320
170	$C_7H_{10}O$ isomer	6550
171	$C_8H_{12}O$ isomer	3210
171	C_6-alkyl benzene + $C_{15}H_{30}$ isomers	215
172	$C_{15}H_{30}$ isomer	710
175	$C_{12}H_{16}$ isomer	T
176	methylbenzofuran isomer	4150
178	cyanobenzene	8760
178	$C_{12}H_{16}$ isomer	T
178	methylbenzofuran isomer	550
179	methylindene isomer	410
180	tolualdehyde isomer	430
180	$C_{12}H_{16}$ isomer	T
181	n-hexadecane	T
181	C_7-alkyl benzene isomer	T
181	phenyl-n-heptane + $C_{16}H_{32}$ isomer	250
182	$C_8H_{12}O$ isomer	T
183	C_7-alkyl benzene isomer	T
184	acetophenone	5160
184	$C_{12}H_{16}$ isomer	2250
184	$C_9H_{13}N$ isomer	T
186	$C_{13}H_{18}$ isomer	T
186	$C_{16}H_{32}$ isomer	T
187	$C_{11}H_{14}$ isomer	T
188	dimethylbenzofuran isomer	2560
188	$C_{13}H_{18}$ isomer	490
188	n-$C_{17}H_{36}$ isomer	T
189	$C_{11}H_{14}$ isomer	38
189	$C_{12}H_{16}$ isomer	T
190	dimethylbenzofuran isomer	2460
191	$C_{17}H_{36}$ isomer	2370
192	$C_{13}H_{18}$ isomer	460
193	$C_{11}H_{12}$ isomer	T
193	$C_{17}H_{36}$ isomer	T
194	$C_{13}H_{18}$ isomer	T
195	d_5-nitrobenzene (es)	
195	$C_{18}H_{36}$ isomer	2030
196	naphthalene	>20000
198	$C_{12}H_{16}$ isomer	NQ
199	$C_{13}H_{18}$ isomer	NQ
200	$C_{14}H_{20}$ isomer	NQ
200	$C_{12}H_{16}$ isomer	2070
200	n-$C_{18}H_{38}$ isomer	170
202	$C_{14}H_{20}$ isomer	1470
202	methylaniline isomer	3250
202	C_2-alkyl aniline isomer	1460
202	$C_{19}H_{40}$ isomer	T
203	2,3-benzothiophene	9590
203	$C_{12}H_{16}$ + n-octadecane	333

(continued)

Table D17 (cont'd)

Elution Temperature (°C)	Compound	ppm
205	$C_{14}H_{20}$ isomer	150
205	$C_{13}H_{18}$ isomer	T
206	$C_{12}H_{14}$ isomer	230
206	$C_{14}H_{20}$ isomer	15
206	C_2-alkyl aniline isomer	1250
207	$C_{14}H_{20}$ isomer	T
208	aniline	150
209	$C_{19}H_{40}$ isomer	T
209	$C_{13}H_{18}$ isomer	NQ
210	methylnaphthalene isomer	9176
210	$C_{15}H_{22}$ isomer	T
211	$C_{14}H_{20}$ isomer	T
211	$C_8H_{11}N$ isomer	2650
212	dimethylphenol isomer	4150
212	$\underline{n}$-$C_{19}H_{40}$ isomer	140
213	$C_8H_{11}N$ isomer	T
214	methylnaphthalene isomer	7615
214	benzylamine	190
215	$C_{15}H_{22}$ isomer	T
215	alkyl-napthalene isomer	736
216	C_3-alkyl phenol isomer	T
217	pentamethylindan isomer	4190
217	$C_{15}H_{22}$ isomer	T
218	$C_{14}H_{20}$ isomer	430
218	$C_{19}H_{38}$ isomer	38
218	methylaniline isomer	40
219	$C_8H_{11}N$ isomer	T
219	$C_{14}H_{10}$ isomer	410
220	ethylnaphthalene isomer	1570
220	phenol + cresol isomer	89600
220	$C_{14}H_{10}$ isomer	560
222	$C_8H_{11}N$ isomer	110
222	ethylnaphthalene isomer	779
222	C_3-alkyl phenol isomer	785
222	dimethylnaphthalene isomer	178
223	$C_{20}H_{40}$ isomer	T
223	C_3-alkyl phenol isomer	990
224	biphenyl	461
224	$C_8H_{11}N$ isomer	2000
224	$C_9H_{13}N$ isomer	50
224	$C_{15}H_{22}$ isomer	T
225	dimethylnaphthalene + C_4-alkyl phenol isomers	620
225	methylquinoline isomer	210
226	C_3-alkyl phenol + dimethyl-naphthalene isomers	7890
226	$\underline{n}$-$C_{20}H_{42}$ + quinoline	5160
227	ethylphenol isomer	2761
227	dimethylphenol isomer	16710
229	C_3-alkyl phenol isomers	6660
229	C_2-alkyl-naphthalene isomer	T
229	$C_9H_{13}N$ isomer	T
229	methylquinoline isomer	T
229	$C_8H_{11}N$ isomer	2140
230	cresol + C_2-alkyl naphthalene isomers	1410
231	C_2-alkyl phenol isomer	1200
231	$C_{20}H_{40}$ isomer	T
232	C_5-alkyl phenol + C_3-alkyl naphthalene isomers	470
232	ethylphenol + methylquinoline isomers (tent.)	4770
233	C_2-alkyl naphthalene isomer	1050
233	C_3-alkyl naphthalene isomer	376
233	dimethylphenol isomer	6150
234	C_3-alkyl phenol isomer	1760
234	C_2-alkyl phenol isomer	1410
234	cresol isomer	410
235	ethylphenol isomer	1270
235	C_2-alkyl naphthalene isomer	T
235	$\underline{n}$-$C_{21}H_{44}$ isomer	87
236	C_3-alkyl naphthalene + C_3-alkyl phenol isomers	1320
236	C_3-alkyl phenol isomer	8210
237	C_3-alkyl phenol isomer	550
237	C_2-alkyl phenol isomer	105100
238	$C_9H_{20}O$ isomer	421
238	$\underline{n}$-$C_{21}H_{42}$ isomer	T
239	C_2-alkyl phenol isomer	75170
239	C_3-alkyl-phenol isomer	1780
239	C_3-alkyl phenol isomer	10500
239	$C_{21}H_{42}$ isomer	T
240	C_3-alkyl phenol isomer	3850
240	C_4-alkyl phenol isomer	T
240	acenaphthene + C_4-alkyl phenol isomer	915
240	C_3-alkyl phenol isomer	5710
240	C_3-alkyl phenol isomer	6720
240	C_4-alkyl phenol isomer	2110
240	C_3-alkyl naphthalene isomer	1570
240	biphenylene	4770

(continued)

Table D17 (cont'd)

Elution Temperature (°C)	Compound	ppm	Elution Temperature (°C)	Compound	ppm
240	C_3-alkyl phenol isomer	1410	240	C_2-alkyl benzaldehyde	8500
240	C_4-alkyl phenol isomer	1710			
240	C_4-alkyl phenol isomer	1350			
240	C_3-alkyl naphthalene isomer	1270			
240	C_3-alkyl phenol isomer	1110			
240	C_4-alkyl phenol isomer	T			
240	dibenzofuran	2760			
240	$C_{16}H_{14}$ isomer	1410			
240	C_4-alkyl phenol isomer	620			
240	C_4-alkyl phenol isomer	2000			
240	fluorene	4140			
240	$C_{13}H_{10}O$ or $C_{14}H_{14}$ isomer	550			
240	triethylbenzene or C_6-alkyl benzene isomer	2180			
240	$C_{10}H_{12}O$ isomer	570			
240	dimethylbenzaldehyde isomer	9970			
240	methylphenanthrene isomer	T			

Table D18. SEMI-VOLATILE ORGANICS IN PROCESS COMPOSITE (-7L) FROM IN SITU COAL GASIFICATION (LLL, ERDA)

Elution Temperature (°C)	Compound	ppm	Elution Temperature (°C)	Compound	ppm
92	CO_2	NQ	136	C_4-alkyl benzene isomer	NQ
96	acetone	NQ	136	n-tridecane	300
96	diethyl ether	NQ	137	C_4-alkyl benzene isomer	57
99	n-nonane	501	138	$C_{13}H_{26}$ isomer	723
99	ethyl acetate	NQ	138	$C_8H_{11}N$ isomer	4761
101	dimethyl ether	NQ	139	n-butylbenzene	1827
102	C_9H_{18} isomer	T	139	$C_8H_{11}N$ isomer	692
103	$C_{10}H_{22}$ + $C_5H_{10}O$ isomers	90	140	$C_{13}H_{26}$ + $C_{14}H_{28}$ isomers	T
104	hydrocarbon (?)	NQ	140	C_4-alkyl benzene isomer	T
105	n-decane	635	141	C_6H_7N isomer	T
105	hydrocarbon (?)	NQ	142	C_4-alkyl benzene isomer	T
106	$C_{10}H_{20}$ isomer	T	142	$C_{13}H_{26}$ isomer	592
107	hydrocarbon	NQ	143	trimethylbenzene isomer	8391
107	toluene	27	143	anisole	47
107	$C_{11}H_{24}$ isomer	371	144	$C_{14}H_{28}$ isomer	49
108	$C_{10}H_{20}$ isomer	538	144	$C_{15}H_{32}$ + C_4-alkyl benzene isomers	293
110	$C_{11}H_{24}$ isomer	47	144	$C_9H_{13}N$ isomer	T
111	$C_6H_{12}O$ (ketone ?) isomer	169	145	C_4-alkyl benzene isomer	T
112	$C_{11}H_{22}$ isomer	T	146	C_6H_8O + $C_{14}H_{30}$ isomers	NQ
113	n-undecane	5976	146	C_8H_{11} isomer	T
115	$C_{11}H_{22}$ isomer	5214	147	indan	6921
115	ethylbenzene	1200	147	acid (?)	NQ
117	xylene + $C_{11}H_{22}$ isomers	694	147	C_6H_7N isomer	NQ
118	$C_{12}H_{26}$ isomer	T	148	C_7H_9N isomer	NQ
120	$C_{12}H_{26}$ isomer	81	149	$C_8H_{11}N$ isomer	NQ
120	$C_{13}H_{28}$ isomer	T	149	$C_9H_{18}O$ isomer	343
121	$C_7H_{14}O$ isomer	97	149	C_4-alkyl benzene isomer	T
122	xylene isomer	684	150	C_5-alkyl benzene isomer	3215
123	n-dodecane	2315	150	n-tetradecane	2976
123	acid (?)	NQ	151	$C_{10}H_{12}$ isomer	T
124	cyclopentanone	NQ	151	$C_8H_{11}N$ isomer	7936
125	n-propylbenzene	T	152	$C_9H_{13}N$ isomer	338
126	$C_{12}H_{24}$ isomer	65	153	n-pentylbenzene	1839
127	ethyltoluene + $C_{12}H_{24}$ isomer	3667	154	$C_{14}H_{28}$ isomer	2761
129	$C_{14}H_{30}$ isomers	T	154	$C_9H_{13}N$ + C_7H_9N isomers (tent.)	NQ
130	C_3-alkyl benzene + $C_{12}H_{24}$ + methylpyridine isomers	3214	155	C_5-alkyl benzene isomer	T
130	$C_{13}H_{26}$ isomer	47	155	$C_{10}H_{15}N$ isomer	3762
132	trimethylbenzene isomer	T	156	C_4-alkyl benzene isomer }	871
132	C_4-alkyl benzene isomer	141	157	$C_{14}H_{28}$ isomer }	
132	n-heptanoic acid	376	157	methyl cresyl ether	476
133	$C_{13}H_{28}$ isomer	T	157	$C_9H_{13}N$ isomer	395
134	$C_8H_{16}O$ isomer	5200	158	$C_9H_{13}N$ isomer	266
135	trimethylbenzene isomer	481	158	$C_{10}H_{15}N$ isomer	265
135	C_2-alkyl pyridine isomer	329	159	$C_{15}H_{30}$ + $C_{14}H_{28}$ isomers	2982
135	$C_{13}H_{28}$ isomer	407			

(continued)

Table D18 (cont'd)

Elution Temperature (°C)	Compound	ppm
162	$C_{10}H_{12}$ isomer	1921
162	$C_7H_{10}O$ isomer	NQ
162	$C_9H_{13}N$ isomer	761
163	C_4-alkyl benzene isomer	2981
163	C_7H_9N isomer	762
164	$C_8H_{11}N$ isomer	871
165	n-pentadecane + $C_{11}H_{14}$ isomer	3989
165	$C_{10}H_{15}N$ isomer	62
166	$C_8H_{11}N$ isomer	31
167	$C_8H_{11}N$ isomer	
167	benzaldehyde	8914
168	$C_{11}H_{14}$ isomer	323
168	C_3-alkyl phenol isomer (tent.)	NQ
170	$C_9H_{13}N$ isomer	411
171	$C_7H_{10}O$ isomer	7921
172	alkyl pyridine isomer	1010
173	$C_8H_{12}O$ isomer	4231
174	$C_{15}H_{30}$ isomer	726
174	alkyl pyridine isomer	NQ
177	$C_{12}H_{16}$ isomer	T
178	$C_9H_{13}N$ isomer	T
178	methylbenzofuran isomer	7828
178	$C_9H_{18}N$ isomer	NQ
179	$C_{16}H_{34}$ isomer	T
179	cyanobenzene + methylbenzofuran isomer	11231
179	C_6H_8O isomer + n-hexadecane	T
180	methylindene isomer	311
180	alkyl pyridine isomer (tent.)	
181	phenyl-n-heptane + $C_{16}H_{34}$ isomer	342
181	acid (?)	NQ
182	benzoic acid	417
183	$C_{16}H_{32}$ + $C_{12}H_{16}$ isomers	62
183	$C_8H_{11}N$ isomer	T
185	acetophenone	9327
186	tetrahydroquinoline	487
187	$C_{13}H_{18}$ isomer	T
187	$C_{16}H_{32}$ isomer	T
187	n-heptadecane	T
189	$C_{11}H_{14}$ isomer	T
189	$C_{12}H_{16}$ isomer	T
189	$C_9H_{13}N$ isomer	620
191	dimethylbenzofuran isomer	4762
193	acid (?)	NQ
195	$C_{11}H_{12}$ isomer	T
195	cresol isomer	NQ
197	d_5-nitrobenzene (es)	
198	naphthalene	72500
199	n-octadecane	476
200	$C_{13}H_{18}$ isomer	T
202	$C_{12}H_{16}$ isomer	2424
204	C_2-alkyl phenol isomer	3740
206	2,3-benzothiophene	11482
206	$C_{19}H_{38}$ isomer	NQ
206	acid (?)	NQ
207	$C_{12}H_{16}$ isomer (tent.)	400
209	$C_{14}H_{20}$ isomer	145
211	$C_{15}H_{22}$ isomer	T
211	methylnaphthalene isomer	11200
211	n-nonadecane	241
212	methylnaphthalene isomer	9200
214	$C_{14}H_{20}$ isomer	500
214	dimethylphenol isomer	4000
215	$C_{19}H_{38}$ isomer	46
217	alkyl-napthalene isomer	876
217	ethylphenol isomer	
218	pentamethylindan + C_3-alkyl phenol isomers	8800
218	$C_{10}H_{15}N$ isomer	47
219	C_3-alkyl phenol isomer	920
221	ethylnaphthalene isomer	811
221	cresol isomer + phenol	62141
222	quinoline or isoquinoline (?)	
222	$C_{15}H_{22}$ isomer	T
223	C_3-alkyl phenol isomer	8210
223	dimethylnaphthalene isomer	277
223	C_3-alkyl phenol isomer	1121
223	n-eicosane	T
226	biphenyl	532
226	methylquinoline isomer	276
227	dimethylnaphthalene + C_4-alkyl phenol isomers	8200
228	dimethylnaphthalene isomer	T
228	C_3-alkyl phenol isomer	5721
229	ethylphenol isomer	2421
230	dimethylphenol isomer	10211
231	cresol isomer	
232	dimethylnaphthalene isomer	T
233	C_3-alkyl naphthalene isomer	421
234	n-heneicosane	96

(continued)

Table D18 (cont'd)

Elution Temperature (°C)	Compound	ppm	Elution Temperature (°C)	Compound
235	C_2-alkyl naphthalene isomer	T		
236	C_3-alkyl phenol isomer	1000		
237	$C_{13}H_{12}$ isomer (tent.)	NQ		
237	dimethylquinoline isomer	326		
238	dimethylphenol isomer	5220		
239	C_3-alkyl naphthalene isomer	1839		
240	C_3-alkyl phenol isomer	2700		
240	dimethylphenol isomer	260		
240	$C_{15}H_{22}$ isomer	NQ		
240	C_3-alkyl phenol isomer	4300		
240	C_4-alkyl phenol isomer	1232		
240	acenaphthene	1100		
240	C_3-alkyl phenol isomer	6250		
240	C_3-alkyl naphthalene + C_3-alkyl phenol isomers	2500		
240	C_4-alkyl phenol isomer	1800		
240	C_4-alkyl phenol isomer	1200		
240	biphenylene	6777		
240	C_3-alkyl phenol isomer	1440		
240	C_3-alkyl phenol isomer	NQ		
240	C_4-alkyl naphthalene isomer	NQ		
240	C_3-alkyl naphthalene isomer	NQ		
240	C_4-alkyl phenol isomer	1000		
240	C_4-alkyl phenol isomer	T		
240	C_3-alkyl naphthalene isomer			
240	dibenzofuran	4391		
240	C_4-alkyl naphthalene isomer	NQ		
240	C_5-alkyl naphthalene isomer	NQ		
240	hydrocarbon (?)	NQ		
240	C_4-alkyl phenol isomer	1435		
240	fluorene	8200		
240	$C_{13}H_{10}O$ or $C_{14}H_{14}$ isomer (?)	NQ		
240	triethylbenzene isomer	1550		
240	C_2-alkyl benzaldehyde (tent.)	10225		
240	C_3-alkyl benzaldehyde (tent.)	4200		
240	tri-sec-butyl phenol isomer	310		
240	$\underline{n}$-$C_{22}H_{46}$ isomer	NQ		
240	$C_{12}H_{11}N$ isomer	NQ		
240	phenylpyridine	NQ		
240	diphenylacetylene	NQ		
240	$\underline{n}$-$C_{23}H_{48}$ isomer	NQ		

Table D19. SEMI-VOLATILE ORGANICS IN WATER (-8L) FROM ENVIRONMENTAL MONITORING WELL #4 DURING IN SITU COAL GASIFICATION (LLL, ERDA)

Elution Temperature (°C)	Compound	ppb	Elution Temperature (°C)	Compound	ppb
101	CO_2	NQ	163	n-decanal	1.5
103	acetaldehyde	NQ	166	acetic acid	73
105	ethyl formate	210	168	benzaldehyde	4.2
106	acetone	NQ	181	unsaturated hydrocarbon (?)	NQ
107	n-butanal	NQ	191	d_5-nitrobenzene (eI)	
107	ethyl acetate	840	204	saturated hydrocarbon	NQ
108	hydrocarbon isomer	33	206	methylnaphthalene isomer (tent.)	T
109	benzene	T	215	phenol	138
110	n-pentanal	T	222	dimethylphenol isomer	646
112	toluene	5.1	223	cresol isomer	607
113	n-hexanal	1.5	229	dimethylphenol isomer	75
123	n-heptanal	0.3	231	C_3-alkyl phenol isomer	T
127	unsaturated hydrocarbon (tent.)	T	233	C_2-alkyl phenol isomer	T
132	n-octanal	4.8	233	ethylphenol isomer	276
150	n-nonanal	10.0	237	C_2-alkyl phenol isomer	246

Table D20. SEMI-VOLATILE ORGANICS IN WATER (-9L) FROM ENVIRONMENTAL MONITORING WELL #5 DURING IN SITU COAL GASIFICATION (LLL, ERDA)

Elution Temperature (°C)	Compound	ppb
112	CO_2	NQ
115	ethyl formate	255
117	ethyl acetate	1320
118	n-pentanal (tent.)	T
118	isopropyl alcohol	522
119	hydrocarbon	NQ
121	toluene	T
127	n-hexanal (tent.)	T
149	n-nonanal	21
155	acetoxy acetone (tent.)	2.4
161	n-decanal	T
164	benzaldehyde	T
166	alcohol (tent.)	16.2
181	$C_8H_{18}O$ (alcohol, tent.)	4.2
187	$C_8H_{18}O$ isomer	3
191	d_5-nitrobenzene (eS)	
216	phenol	159
222	dimethylphenol isomer	570
222	ethylphenol isomer	T
225	cresol isomer	96
229	C_3-alkyl phenol isomer	T
230	C_2-alkyl phenol isomer	43
232	C_3-alkyl phenol isomer	T
233	C_2-alkyl phenol isomer	150
233	ethylphenol isomer	T
236	ethylphenol isomer	T

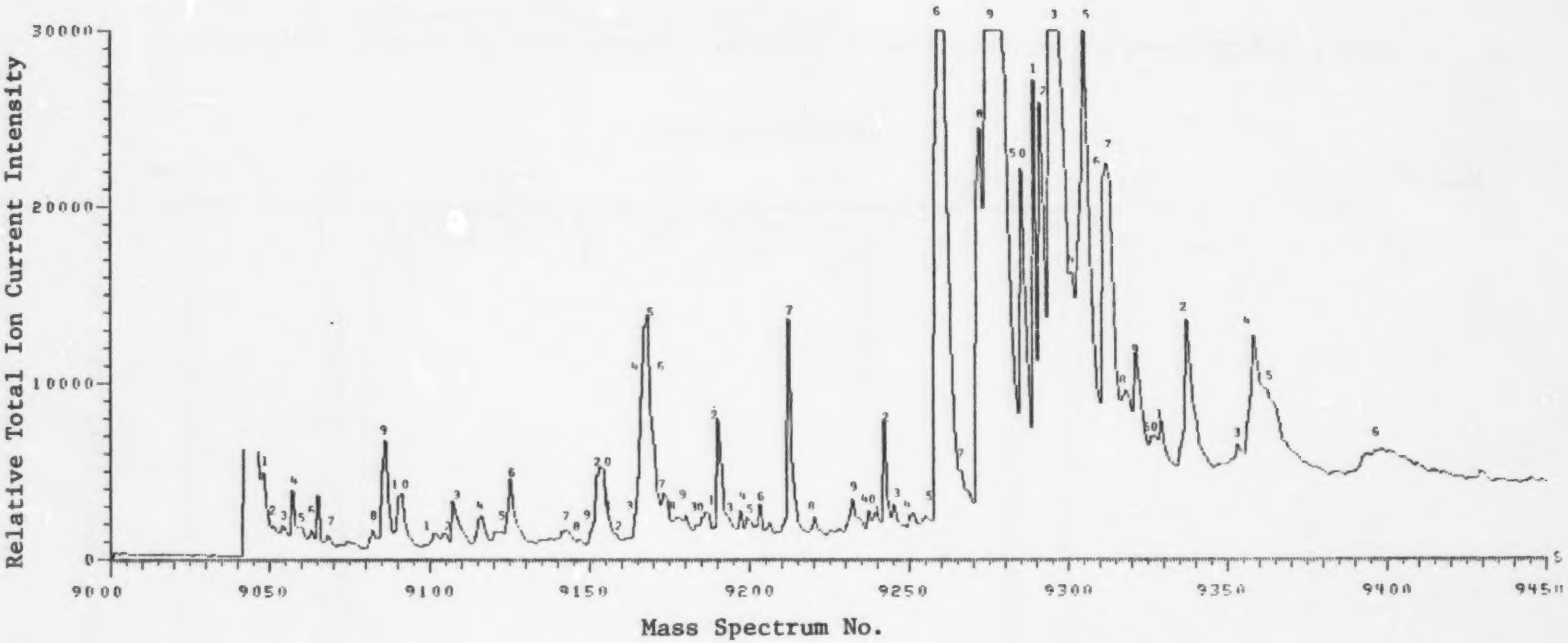


Figure D10. Profile of semi-volatile organics in neutral fraction of water sample (-10L) from dewatering well #4 (LLL, ERDA).

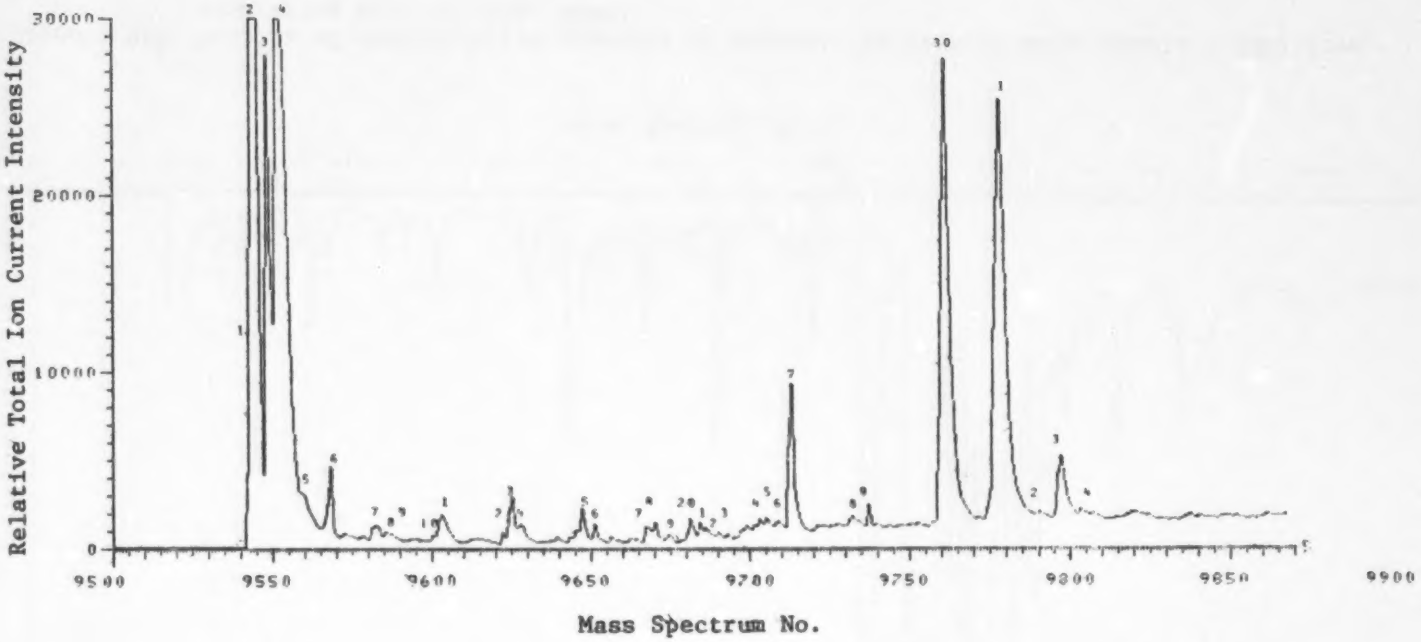


Figure D11. Profile of semi-volatile organics in acid fraction of water sample (-10L) from dewatering well #4 (LLL, ERDA).

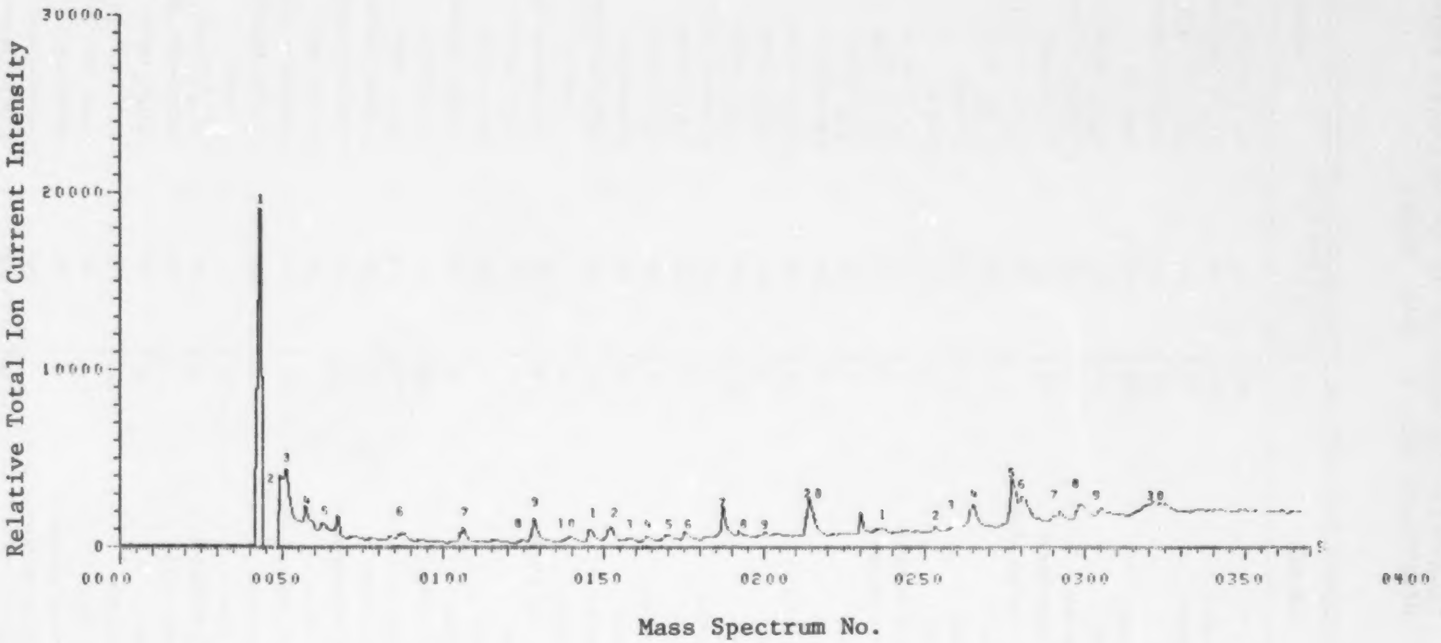


Figure D12. Profile of semi-volatile organics in basic fraction of water sample (-10L) from dewatering well #4 (LLL, ERDA).

Table D21. SEMI-VOLATILE ORGANICS IN WATER (-10L) FROM DEWATERING WELL #4 (LLL, ERDA)

Elution Temperature (°C)	Compound	ppb	Elution Temperature (°C)	Compound	ppb
101	CO_2	NQ	142	indan or C_9H_{10} isomer	T
102	diethyl ether	NQ	142	$C_8H_{16}O_2$ acid isomer	1.2
103	acetaldehyde	NQ	144	n-octanoic acid	33
105	acetone	NQ	144	methylcyclopentenone isomer	37
105	ethyl formate	369	145	n-nonanal	25
106	n-butanal	NQ	147	$C_{10}H_{18}$ isomer (tent.)	T
106	ethyl acetate	NQ	152	C_2-alkyl cyclopentenone	20
106	methyl ethyl ketone	NQ	154	$C_9H_{18}O$ isomer	9
107	benzene + methyl isopropyl		155	n-nonanoic acid	9.6
	ketone	3	155	$C_{10}H_{12}$ isomer	T
109	2-pentanone	27	157	n-decanal	T
110	n-pentanal	T	157	indene	T
110	4-methyl-2-pentanone	T	158	$C_8H_{12}O$ isomer	58
111	3-methyl-2-pentanone	3	159	$C_9H_{14}O$ isomer	T
112	toluene	T	163	C_6H_8O isomer	T
113	3-hexanone	T	164	benzaldehyde	T
114	n-pentanoic acid	64	164	$C_7H_{10}O$ isomer	160
115	n-hexanal	T	165	$C_7H_{10}O$ isomer	167
115	2-hexanone	0.6	166	$C_8H_{12}O$ isomer	154
117	ethylbenzene	T	167	n-decanoic acid	1.2
118	p-xylene	T	168	$C_7H_{10}O$ isomer	9
119	$C_7H_{14}O$ isomer	T	168	$C_9H_{14}O$ isomer	T
120	3-heptanone	T	169	n-undecanal	4.2
121	n-hexanoic acid	2.4	170	methylbenzofuran isomer	
122	2-heptanone	3		(tent.)	T
123	$C_6H_{12}O_2$ acid isomer	T	171	cyanobenzene (tent.)	T
123	o-xylene	T	173	phenyl acetate	10
124	n-heptanal	1.8	174	benzoic acid	1.8
124	$C_7H_{12}O$ isomer	T	174	C_3-alkyl pentenone isomer	10.2
124	cyclopentanone	45	176	acetophenone	107
125	2-methylcyclopentanone	9	178	$C_9H_{14}O$ isomer	T
126	isopropylbenzene	T	179	p-cresyl acetate (tent.)	T
126	3-methylcyclopentanone	25	180	methylacetophenone isomer	9
127	$C_7H_{12}O$ isomer	6.6	181	o-toluic acid	T
130	C_3-alkyl benzene isomer	T	181	unsaturated hydrocarbon	T
130	$C_7H_{12}O$ isomer	T	182	C_2-alkyl benzofuran isomer	
131	$C_8H_{16}O$ isomer	3		(tent.)	T
132	trimethylbenzene isomer	T	183	$C_9H_{10}O_2$ isomer	0.6
132	n-heptanoic acid	29	185	methylacetophenone isomer	0.6
133	n-octanal	13	185	$C_9H_{10}O_2$ isomer	1.2
135	cyclohexanone	16	189	d_5-nitrobenzene (sS)	
136	$C_7H_{12}O$ isomer	4.8	189	toluic acid isomer	2.4
138	1,2,3-trimethylbenzene	T	189	naphthalene	46
139	C_2-alkyl cyclopentenone isomer		196	benzothiophene	3
	(tent.)	9	198	$C_{10}H_{12}O_2$ isomer	3.6
141	C_2-alkyl cyclopentenone isomer	4.2	201	β-methylnaphthalene	4.2

(continued)

Table D21 (cont'd)

Elution Temperature (°C)	Compound	ppb	Elution Temperature (°C)	Compound
202	saturated hydrocarbon (?)	NQ		
203	dimethylphenol isomer	120		
205	α-methylnaphthalene	3		
207	C_3-alkyl phenol isomer	9		
211	cresol isomer	1056		
212	C_3-alkyl phenol isomer	T		
213	phenol	120		
215	C_4-alkyl phenol isomer	T		
218	C_2-alkyl phenol isomer	18.6		
220	cresol isomer	594		
225	C_3-alkyl phenol isomer	120		
227	C_2-alkyl phenol isomer	141		
228	C_3-alkyl phenol isomer	135		
229	C_2-alkyl phenol isomer	34		
230	C_2-alkyl phenol isomer	436		
232	ethylphenol isomer	47		
232	C_4-alkyl phenol isomer	T		
233	C_3-alkyl phenol isomer	23		
235	C_2-alkyl phenol isomer	40		
236	C_2-alkyl phenol isomer	147		
239	C_3-alkyl phenol isomer	119		
240	C_3-alkyl phenol isomer	124		
240	C_4-alkyl phenol isomer	9		
240	C_3-alkyl phenol isomer	47		
240	C_3-alkyl phenol isomer	3		
240	C_4-alkyl phenol isomer	6.6		
240	unknown	NQ		
240	ethylbenzaldehyde isomer	157		
240	C_5-alkyl phenol isomer	3		
240	3,4-dimethylbenzaldehyde	150		
240	C_3-alkyl benzaldehyde isomer (tent.)	360		

Table D22. SEMI-VOLATILE ORGANICS IN WATER (-11L) FROM DEWATERING WELL #5 (LLL, ERDA)

Elution Temperature (°C)	Compound	ppb	Elution Temperature (°C)	Compound	ppb
112	CO_2	NQ	141	hydrocarbon (tent.)	T
115	acetone	NQ	148	aldehyde (tent.)	NQ
116	acetaldehyde	NQ	151	n-nonanal	41
117	ethyl formate	615	162	n-decanal + indene (tent.)	9
117	isopropanol	94	173	acetic acid	T
118	ethyl acetate	1092	191	d_5-nitrobenzene (eS)	
118	benzene + saturated hydrocarbon	T	216	phenol	141
			222	dimethylphenol isomer	339
119	n-pentanal	4.2	223	cresol isomer	263
121	toluene	130	228	C_3-alkyl phenol isomer	T
123	n-hexanal	T	230	dimethylphenol isomer	14
132	C_5H_8O isomer	T	233	C_2-alkyl phenol isomer	T
133	n-heptanal	T	234	ethylphenol isomer	186
141	n-octanal	9			

Table D23. SEMI-VOLATILE ORGANICS IN WATER (-12L) FROM ENVIRONMENTAL MONITORING WELL #1 AFTER IN SITU COAL GASIFICATION (LLL, ERDA)

Elution Temperature (°C)	Compound	ppb	Elution Temperature (°C)	Compound	ppb
102	CO_2	NQ	166	benzaldehyde	T
106	acetaldehyde + diethyl ether	NQ	175	$C_{10}H_{20}O$ isomer (decanal ?)	2.4
109	C_9H_{20} isomer	T	176	unsaturated hydrocarbon	T
109	ethyl formate	930	188	methyl propyl ketene (?)	33
109	ethyl acetate	233	189	d_5-nitrobenzene (es)	
111	n-decane	10	192	naphthalene	47
112	n-pentanal	T	216	phenol	27
112	$C_{11}H_{24}$ isomer (tent.)	T	220	dimethyl phenol isomer	274
114	toluene	42	223	cresol isomer	239
117	n-hexanal	6.6	227	C_3-alkyl phenol isomer	T
118	n-undecane	T	228	ethylphenol isomer	10
126	n-heptanal	T	231	C_2-alkyl phenol isomer	163
148	n-nonanal	7.2	232	ethylphenol isomer	58
155	acetoxy acetone (tent.)	NQ	236	C_3-alkyl phenol isomer	T
156	$C_7H_{12}O$ isomer (tent.)	1.8	237	C_2-alkyl phenol isomer	13
160	$C_8H_{16}O$ isomer (tent.)	0.6	238	C_3-alkyl phenol isomer	T

Table D24. SEMI-VOLATILE ORGANICS IN WATER (-13L) FROM ENVIRONMENTAL MONITORING WELL #4 AFTER *IN SITU* COAL GASIFICATION (LLL, ERDA)

Elution Temperature (°C)	Compound	ppb	Elution Temperature (°C)	Compound	ppb
101	CO_2	NQ	182	acetoxy acetone (tent.)	NQ
103	acetaldehyde	NQ	188	d_5-nitrobenzene (es)	
105	ethyl formate	NQ	213	phenol	93
106	ethyl acetate	NQ	220	dimethylphenol isomer	390
106	acetone	NQ	221	cresol isomer	388
110	*n*-butanal (tent.)	NQ	226	dimethylphenol isomer	22
111	*n*-pentanal	NQ	227	ethylphenol isomer	73
113	toluene	T	230	ethylphenol isomer	261
113	$C_5H_{10}O_2$ isomer (tent.)	T	231	C_2-alkyl phenol isomer	79
116	*n*-hexanal	T	235	C_2-alkyl phenol isomer	6.6
148	*n*-nonanal	66	238	C_4-alkyl phenol isomer (tent.)	T

Table D25. SEMI-VOLATILE ORGANICS IN WATER (-14L) FROM ENVIRONMENTAL MONITORING WELL #2 AFTER *IN SITU* COAL GASIFICATION (LLL, ERDA)

Elution Temperature (°C)	Compound	ppb	Elution Temperature (°C)	Compound	ppb
101	CO_2	NQ	154	unsaturated hydrocarbon	8.4
103	diethyl ether	NQ	157	methyl acetoacetate (tent.)	25
103	acetaldehyde	NQ	159	*n*-decanal	34
105	ethyl formate	NQ	165	benzaldehyde	T
105	acetone	NQ	185	unknown	NQ
106	ethyl acetate	NQ	190	d_5-nitrobenzene (e[illegible])	
107	*n*-nonane (tent.)	T	196	unknown	NQ
110	*n*-butanal	NQ	205	acetic acid (tent.)	T
111	hydrocarbon	NQ	215	phenol	232
112	*n*-decane (tent.)	T	217	unknown	NQ
112	toluene (tent.)	15	221	dimethylphenol isomer	753
117	*n*-hexanal	T	222	cresol isomer	793
119	hydrocarbon (?)	T	228	C_2-alkyl phenol isomer	46
126	*n*-heptanal	28	231	dimethylphenol isomer	339
138	*n*-octanal	T	232	ethylphenol isomer	73
146	$C_9H_{18}O$ isomer	T	237	C_2-alkyl phenol isomer	9
148	*n*-nonanal	39			

Table D26. SEMI-VOLATILE ORGANICS IN LIQUID (-15T) FROM PRODUCTION WELL #1 AFTER IN SITU COAL GASIFICATION (LLL, ERDA)

Elution Temperature (°C)	Compound	ppm	Elution Temperature (°C)	Compound	ppm
92	CO_2	NQ	223	phenol	10
97	acetone	NQ	227	$C_{20}H_{40}$ isomer	T
99	hydrocarbon (tent.)	T	231	dimethylphenol isomer	1510
195	$C_{19}H_{40}$ isomer	T	232	cresol isomer	2110
196	d_5-nitrobenzene (eS)		233	n-$C_{21}H_{44}$	T
198	n-octadecane (tent.)	20			
208	$C_{19}H_{40}$ isomer	T	238	dimethylphenol isomer	17
210	n-nonadecane	2100	240	ethylphenol isomer	46
215	$C_{19}H_{38}$ isomer (tent.)	15	240	C_2-alkyl phenol isomer	14
217	$C_{20}H_{42}$ isomer	50	240	C_3-alkyl phenol isomer	T
219	$C_{20}H_{40}$ isomer	11	240	C_2-alkyl phenol isomer	T
220	$C_{20}H_{42}$ isomer	T	240	$C_{14}H_{10}$ isomer	T
222	n-$C_{20}H_{42}$	2615			

Table D27. SEMI-VOLATILE ORGANICS IN WATER (-16L) FROM DEWATERING WELL #4 AFTER IN SITU COAL GASIFICATION (LLL, ERDA)

Elution Temperature (°C)	Compound	ppb	Elution Temperature (°C)	Compound	ppb
102	CO_2	NQ	205	α-methylnaphthalene	T
103	acetaldehyde	NQ	208	unsaturated hydrocarbon	T
105	ethyl formate	720	213	cresol isomer	6.6
105	acetone	NQ	214	phenol	163
107	n-butanal	NQ	217	dimethylnaphthalene isomer	T
108	hydrocarbon	T	219	ethylphenol isomer	T
108	ethyl acetate	1185	220	dimethylphenol isomer	186
108	n-pentanal	T	222	cresol isomer	153
112	toluene	26	223	dimethylphenol isomer	34
113	n-hexanal	3.6	224	ethylphenol isomer	183
115	$C_4H_8O_2$ isomer	T	224	cresol isomer	129
116	hydrocarbon (tent.)	T	225	C_3-alkyl phenol isomer	9
120	n-heptanal	6	227	C_2-alkyl phenol isomer	T
123	cyclopentanone	T	229	C_3-alkyl phenol isomer	T
129	n-octanal	3	233	ethylphenol isomer	120
189	d_5-nitrobenzene (sm)		233	acenaphthene	T
190	naphthalene	T	234	C_4-alkyl phenol isomer	T
202	β-methylnaphthalene	T	237	C_3-alkyl phenol isomer	T
203	dimethylphenol isomer	T			

Table D28. SEMI-VOLATILE ORGANICS IN WATER (-17L) FROM DEWATERING WELL #5 AFTER IN SITU COAL GASIFICATION (LLL, ERDA)

Elution Temperature (°C)	Compound	ppb	Elution Temperature (°C)	Compound	ppb
103	CO_2	NQ	188	methyl propyl ketone (tent.)	NQ
104	diethyl ether	NQ	189	d_5-nitrobenzene (eS)	
105	acetaldehyde	NQ	214	phenol	59
107	ethyl formate	210	215	alcohol (tent.)	NQ
108	hydrocarbon	3	220	dimethylphenol isomer	450
109	ethyl acetate	1479	222	cresol isomer	257
113	toluene	T	227	C_2-alkyl phenol isomer	T
114	*n*-pentanal (tent.)	T	229	C_2-alkyl phenol isomer	19
117	*n*-hexanal	T	230	ethylphenol isomer	279
135	*n*-octanal	T	235	C_3-alkyl phenol isomer	T
138	alcohol	NQ			

Table D29. SEMI-VOLATILE ORGANICS IN WATER (-18L) FROM DEWATERING WELL #4 AFTER IN SITU COAL GASIFICATION (LLL, ERDA)

Elution Temperature (°C)	Compound	ppb
92	CO_2	NQ
95	acetaldehyde	NQ
97	ethyl formate	866
99	ethyl acetate	1725
100	dimethyl ether	NQ
108	toluene	126
110	n-pentanoic acid	138
111	n-hexanal (tent.)	T
120	n-hexanoic acid	132
134	n-heptanoic acid	145
142	pentafluoropropionyl derivative (unknown)	NQ
147	n-octanoic acid	120
161	hydrocarbon	33
166	$C_8H_{12}O$ (cyclic ketone ?)	16
173	$C_7H_{10}O$ (ketone ?)	67
175	$C_8H_{12}O$ isomer	T
177	$C_7H_{10}O$ isomer	T
177	$C_7H_{10}O$ isomer	T
187	acetophenone	33
196	d_5-nitrobenzene (eS)	
199	naphthalene	T
202	methylaniline isomer or C_7H_9N	33
209	aniline	12
215	dimethylphenol isomer	17
221	C_3-alkyl phenol isomer	T
222	phenol	13
224	cresol isomer	1572
225	C_3-alkyl phenol isomer	T
229	ethylphenol isomer	T
230	dimethylphenol isomer	T
232	ethylphenol isomer	3
232	cresol isomer	1548
233	dimethylphenol isomer	1560
234	dimethylphenol isomer	9
235	cresol isomer	T
236	C_3-alkyl phenol isomer	T
237	C_3-alkyl phenol isomer	T
238	C_2-alkyl phenol isomer	T
239	C_3-alkyl phenol isomer	10
240	C_2-alkyl phenol isomer	15
240	C_3-alkyl phenol isomer	1075
240	C_3-alkyl phenol isomer	863
240	C_4-alkyl phenol isomer	T
240	C_3-alkyl phenol isomer	3
240	C_3-alkyl phenol isomer	5.4
240	C_3-alkyl phenol isomer	6.6
240	C_4-alkyl phenol isomer	T
240	C_2-alkyl phenol isomer	T
240	C_3-alkyl phenol isomer	T
240	C_3-alkyl phenol isomer	T

Table D30. SEMI-VOLATILE ORGANICS IN WATER (-19L) FROM PRODUCTION WELL #1 AFTER IN SITU COAL GASIFICATION (LLL, ERDA)

Elution Temperature (°C)	Compound	ppb	Elution Temperature (°C)	Compound	ppb
92	CO_2	NQ	164	acetic acid	16
96	acetaldehyde	NQ	196	d_5-nitrobenzene (eS)	
97	ethyl formate	NQ	226	phenol	45
99	ethyl acetate	NQ	231	ethylphenol isomer	T
101	dimethyl ether	NQ	232	dimethylphenol isomer	90
101	hydrocarbon (?)	8.4	233	cresol isomer	126
109	toluene	150	235	C_2-alkyl phenol isomer	T
111	hydrocarbon (tent.)	9	235	C_3-alkyl phenol isomer	9
112	$C_6H_{12}O_2$ isomer (tent.)	11	236	cresol isomer	T
123	aldehyde (?)	NQ	239	C_2-alkyl phenol isomer	13
137	n-octane	T	240	C_2-alkyl phenol isomer	16
141	hydrocarbon (tent.)	T	240	C_3-alkyl phenol isomer	T
151	n-nonanal	16	240	C_2-alkyl phenol isomer	T
159	acetol acetate (?)	NQ	240	ethylphenol isomer	10
161	unknown	NQ	240	C_3-alkyl phenol isomer	T

Table D31. SEMI-VOLATILE ORGANICS IN WATER (~20L) FROM PRODUCTION WELL #1 AFTER *IN SITU* COAL GASIFICATION (LLL, ERDA)

Elution Temperature (°C)	Compound	ppb	Elution Temperature (°C)	Compound	ppb
92	CO_2	NQ	196	d_5-nitrobenzene (e#)	
97	acetone	NQ	211	hydrocarbon (?)	T
97	ethyl formate	546	222	hydrocarbon (?)	T
99	ethyl acetate	1209	224	phenol	T
100	hydrocarbon (?)	T	229	cresol isomer	T
101	dimethyl ether	NQ	230	ethyl phenol isomer	T
102	hydrocarbon (?)	T	231	dimethylphenol isomer	T
105	*n*-pentanal	T	233	dimethylphenol isomer	T
109	toluene	9.0	233	cresol isomer	T
111	*n*-hexanal	T	234	C_3-alkyl phenol isomer	T
114	hydrocarbon (?)	T	239	dimethylphenol isomer	T
122	*n*-heptanal	3.0	240	C_3-alkyl phenol isomer	T
136	*n*-octanal	10	240	dimethylphenol isomer	45
150	*n*-nonanal	39	240	ethylphenol isomer	49
161	hydrocarbon (?)	9	240	C_3-alkyl phenol isomer	T
173	acetic acid	T	240	$C_{14}H_{10}$ isomer (tent.)	T
183	hydrocarbon (?)	NQ			

Table D32. SEMI-VOLATILE ORGANICS IN TAR (-1L) FROM IN SITU COAL GASIFICATION DURING HANNA #2, PHASE I (LERC, ERDA)[a]

Elution Temperature (°C)	Compound
92	CO_2
97	hydrocarbon (unknown)
97	ethyl formate
98	acetone
99	ethyl acetate
101	n-nonane
101	dimethyl ether
102	C_9H_{18} isomer
103	$C_{10}H_{22}$ isomer
104	C_9H_{18} isomer
105	$C_{10}H_{20}$ isomer
106	n-decane
108	$C_{10}H_{20}$ isomer
109	toluene
110	$C_{11}H_{24}$ isomer
111	$C_6H_{12}O$ isomer
111	$C_{10}H_{20}$ isomer
112	$C_{11}H_{22}$ isomer
113	n-undecane
115	$C_{11}H_{22}$ isomer
115	ethylbenzene
115	$C_{11}H_{22}$ isomer
117	xylene isomer
119	xylene isomer
120	$C_{12}H_{26}$ isomer
120	$C_{11}H_{22}$ isomer
122	$C_{13}H_{28}$ + C_3-alkyl benzene isomer
122	$C_7H_{14}O$ ketone isomers
123	n-dodecane
124	xylene isomer
126	n-propylbenzene
127	$C_{12}H_{24}$ isomer
128	ethyltoluene isomer
130	$C_{14}H_{30}$ isomer
130	trimethylbenzene isomer
131	$C_{12}H_{24}$ isomer
131	$C_{13}H_{26}$ isomer
132	styrene
133	$C_{13}H_{28}$ isomer
133	C_3-alkyl benzene isomer
134	$C_{13}H_{26}$ isomer
134	C_4-alkyl benzene isomer
135	$C_8H_{16}O$ ketone isomer (tent.)
136	trimethylbenzene isomer + n-tridecane
138	C_4-alkyl benzene isomer
139	C_4-alkyl benzene isomer
139	$C_{13}H_{26}$ isomer
140	n-butylbenzene
140	$C_{14}H_{28}$ isomer
141	C_4-alkyl benzene isomer
142	C_5-alkyl benzene isomer
142	$C_{13}H_{26}$ isomer
144	trimethylbenzene isomer
146	C_4-alkyl benzene isomer
146	methylstyrene
147	$C_{15}H_{32}$ isomer
148	C_4-alkyl benzene isomer
149	indan or C_9H_{10} isomer
149	$C_9H_{18}O$ isomer
150	n-tetradecane
152	C_5-alkyl benzene isomer
152	methylindan or $C_{10}H_{12}$ isomer
153	C_5-alkyl benzene isomer
154	n-pentylbenzene + $C_{14}H_{28}$ isomer
155	$C_{16}H_{34}$ isomer
156	C_5-alkyl benzene isomer
156	$C_{14}H_{28}$ + C_4-alkyl benzene isomers
159	C_5-alkyl benzene isomer
160	C_6-alkyl benzene isomer
160	$C_{14}H_{28}$ + $C_{10}H_{22}$ isomers
161	$C_{15}H_{32}$ isomer
162	$C_{15}H_{30}$ isomer
163	n-pentadecane + $C_{10}H_{12}$ isomer
164	indene
165	C_4-alkyl benzene isomer
166	benzofuran + $C_{11}H_{14}$ isomers
166	$C_{10}H_{12}$ isomer
167	$C_{11}H_{14}$ isomer
167	phenyl-n-hexane
168	$C_{15}H_{30}$ isomer
169	$C_{11}H_{14}$ isomer
170	C_6-alkyl benzene isomer
171	$C_{15}H_{10}$ isomer
171	$C_7H_{10}O$ isomer
172	$C_8H_{12}O$ isomer
172	$C_{15}H_{28}$ isomer (tent.)
173	hydrocarbon (unknown)
174	C_5-alkyl benzene isomer

(continued)

Table D32 (cont'd)

Elution Temperature (°C)	Compound
175	$C_{11}H_{14}$ isomer
177	$C_{11}H_{14}$ isomer + n-hexadecane
177	methylindene isomer
178	methylbenzofuran isomer
180	methylbenzofuran isomer
181	methylindene isomer
182	phenyl-n-heptane + $C_{16}H_{32}$ isomer
182	$C_{12}H_{16}$ isomer
184	$C_{11}H_{14}$ isomer
187	C_9-alkyl benzene isomer
188	$C_{13}H_{18}$ + $C_{17}H_{36}$ isomers
189	dimethylbenzofuran isomer
190	$C_{12}H_{16}$ isomer
191	$C_{11}H_{12}$ or methyldihydronaphthalene + $C_{13}H_{18}$ isomers
192	dimethylbenzofuran isomer
193	$C_{13}H_{18}$ isomer
194	$C_{11}H_{12}$ isomer
195	n-nonadecane
196	$C_{11}H_{12}$ isomer + phenyl-n-octane
197	d_5-nitrobenzene (eS)
198	naphthalene
199	hydrocarbon (unknown)
200	$C_{14}H_{20}$ isomer
201	$C_{11}H_{12}$ isomer
201	methylaniline + C_2-alkyl aniline isomers
202	$C_{12}H_{16}$ isomer
203	$C_{12}H_{16}$ isomer
204	$C_{20}H_{42}$ isomer
205	2,3-benzothiophene
206	$C_{21}H_{42}$ isomer
208	$C_{15}H_{22}$ isomer
208	aniline
209	hydrocarbon (unknown)
210	$C_{15}H_{22}$ isomer (tent.)
210	n-nonadecane
211	methylnaphthalene isomer
211	C_2-alkyl aniline isomer
212	hydrocarbon (unknown)
213	$C_{15}H_{22}$ isomer
214	dimethylphenol isomer
214	benzylamine or methylaniline
215	$C_{14}H_{20}$ isomer
216	methylnaphthalene isomer
216	C_7H_9N isomer
217	$C_{14}H_{10}$ isomer
219	pentamethylindan isomer
220	C_3-alkyl phenol isomer
221	$C_{19}H_{38}$ isomer
221	cresol isomer
221	C_2-alkyl aniline isomer
221	phenol
222	ethylnaphthalene isomer
222	quinoline
222	cresol isomer
223	$C_{15}H_{22}$ isomer
223	methylquinoline isomer
224	n-eicosane
225	dimethylnaphthalene isomer
225	C_3-alkyl phenol isomer
227	biphenyl
228	ethylphenol isomer
229	dimethylnaphthalene isomer
229	dimethylphenol isomer
230	dimethylnaphthalene isomer
230	cresol isomer
231	cresol isomer
232	ethylphenol isomer
233	dimethylphenol isomer
233	C_3-alkyl phenol isomer
235	dimethylnaphthalene isomer
235	C_3-alkyl phenol isomer
235	methylquinoline + methylphenanthrene isomers
236	C_3-alkyl naphthalene isomer
237	n-heneicosane
237	C_2-alkyl phenol isomer
237	C_2-alkyl quinoline isomer
238	dimethylnaphthalene isomer
238	dimethylphenol isomer
239	C_3-alkyl phenol isomer
240	C_3-alkyl phenol isomer
240	C_4-alkyl naphthalene isomer
240	C_3-alkyl naphthalene isomer
240	C_2-alkyl phenol isomer
240	C_3-alkyl phenol isomer

(continued)

Table D32 (cont'd)

Elution Temperature (°C)	Compound	Elution Temperature (°C)	Compound
240	C_2-alkyl phenol tri-sec-butylphenol isomers		
240	C_3-alkyl naphthalene isomer		
240	C_4-alkyl naphthalene isomer		
240	acenaphthene		
240	C_4-alkyl phenol isomer		
240	C_3-alkyl phenol isomer		
240	C_3-alkyl phenol isomer		
240	C_3-alkyl naphthalene isomer		
240	tributylphenol isomer		
240	C_4-alkyl phenol isomer		
240	biphenylene		
240	C_3-alkyl phenol isomer		
240	C_5-alkyl naphthalene + C_3-alkyl phenol isomers		
240	C_5-alkyl naphthalene isomer		
240	C_3-alkyl naphthalene isomer		
240	C_4-alkyl phenol isomer		
240	C_5-alkyl naphthalene isomer		
240	dibenzofuran		
240	C_4-alkyl phenol isomer		
240	hydrocarbon (unknown)		
240	alkyl phenol		
240	$C_{14}H_{10}$ isomer		
240	fluorene		
240	C_8-alkyl phenol isomer (tent.)		
240	C_2-alkyl quinoline isomer		

---

[a] Sample was not quantitated, since it had been collected and stored for several months before analysis.

Table D33. SEMI-VOLATILE ORGANICS IN WATER (-2L) FROM WELL #5, HANNA #2 (LERC, ERDA)

Elution Temperature (°C)	Compound	ppb	Elution Temperature (°C)	Compound	ppb
93	CO_2	NQ	187	$C_{17}H_{36}$ isomer	5.4
104	hydrocarbon (unknown)	NQ	193	*n*-heptadecane	10.8
107	aldehyde (unknown)	NQ	196	$C_{17}H_{34}$ isomer	T
112	toluene	T	203	d_5-nitrobenzene (eI)	
114	*n*-hexanal	T	205	*n*-octadecane	13
116	hydrocarbon (unknown)	NQ	206	hydrocarbon (unknown)	NQ
127	hydrocarbon (unknown)	NQ	217	*n*-nonadecane	4.2
127	*n*-heptanal	3	217	methylnaphthalene isomer	29
140	hydrocarbon (unknown)	NQ	230	phenol	22
141	*n*-octanal	7.2	231	$C_{12}H_{10}$ isomer (tent.)	T
146	*n*-tridecane	16.2	233	C_2-alkyl naphthalene isomer	1.2
153	*n*-tetradecane	11.4	235	hydrocarbon (unknown)	NQ
154	aldehyde (tent.)	13.8	238	dimethylphenol isomer	279
155	*n*-nonanal	33	239	cresol isomer	192
166	*n*-pentadecane	10.8	240	dimethylphenol isomer	T
169	*n*-decanal	12.6	240	dimethylphenol isomer	17
169	$C_{15}H_{30}$ isomer	2.4	240	C_3-alkyl phenol isomer	T
171	hydrocarbon (unknown)	NQ	240	C_3-alkyl phenol isomer	T
173	hydrocarbon (unknown)	NQ	240	ethylphenol isomer	35
180	*n*-hexadecane	10.2	240	ethylphenol isomer	33
181	$C_{17}H_{36}$ isomer	1.8	240	C_3-alkyl phenol isomer	T
183	$C_{15}H_{30}$ isomer (tent.)	T	240	C_2-alkyl phenol isomer	4.8

Table D34. SEMI-VOLATILE ORGANICS IN WATER (-3L) FROM WELL #6, HANNA #2 (LERC, ERDA)

Elution Temp. (°C)	Compound	ppb	Elution Temp. (°C)	Compound	ppb
94	n-butanal	NQ	150	$C_7H_{16}O$ isomer	T
94	acetone	NQ	151	2-ethyl-1-hexanol	53
95	C_7H_{16} isomer (tent.)	T	152	$C_9H_{18}O$ isomer	17
95	benzene	15	186	d_5-nitrobenzene (eS)	
97	n-pentanal	7.2	213	phenol	207
99	C_8H_{18} isomer (tent.)	9	214	cresol isomer	50
99	toluene	T	221	dimethylphenol isomer	246
102	methylbutanal isomer	6.6	225	cresol isomer	32
102	n-hexanal	T	229	cresol isomer	11
117	n-heptanal	23	231	dimethylphenol isomer	55
119	cyclopentanone	T	233	C_3-alkyl phenol isomer	T
120	$C_8H_{16}O$ isomer	1.2	234	dimethyl phenol isomer	126
128	2-octanone (tent.)	4.8	235	ethylphenol isomer	122
130	n-octanal	T	239	C_3-alkyl phenol isomer	T
147	n-heptanol	14	240	C_2-alkyl phenol isomer	55
147	methylcyclohexanol	T			

Table D35. SEMI-VOLATILE ORGANICS IN WATER (-4L) FROM WELL #6, HANNA #2 (LERC, ERDA)

Elution Temperature (°C)	Compound	Elution Temperature (°C)	Compound
No semi-volatiles were detected, detection limit was ~1 ppb.			

Table D36. SEMI-VOLATILES ORGANICS IN WATER (-5L) FROM WELL #5, HANNA #2 (LERC, ERDA)

Elution Temp. (°C)	Compound	ppb	Elution Temp. (°C)	Compound	ppb
98	benzene	T	116	$C_8H_{16}O$ isomer (tent.)	T
99	$C_5H_{10}O$ isomer (tent.)	7.8	127	methylheptanone	T
100	n-pentanal	22	128	n-octanal (tent.)	T
101	C_7H_{16} isomer (tent.)	3	131	$C_7H_{16}O$ isomer	T
102	methylbutanal isomer	T	142	n-nonanal	T
104	C_7H_{16} isomer	T	148	$C_6H_{10}O_2$ isomer (tent.) + $C_6H_{14}O$ isomer (tent.)	49
106	toluene	T	155	2-ethyl-1-hexanol	29
108	n-hexanal + C_8H_{18} isomer	T	159	benzaldehyde	T
111	C_9H_{20} isomer (tent.)	1.8	187	d_5-nitrobenzene (eW)	
112	C_9H_{18} isomer (tent.)	T	215	phenol	32
114	$C_7H_{14}O$ isomer (tent.)	T	229	C_2-alkyl phenol isomer	46
115	n-heptanal	97			

Table D37. SEMI-VOLATILE ORGANICS IN PRODUCT WATER SAMPLE #1 (-8L) FROM WELL 5-6 IN SITU COAL GASIFICATION (LERC)

Elution Temperature (°C)	Compound[a]	ppb	Elution Temperature (°C)	Compound	ppb
100	methyl ethyl ketone	9	173	C_7H_{12} isomer	3
104	2-pentanone	13.8	174	benzonitrile	T
105	$C_5H_{10}O_2$ (carboxylic acid)	18	175	C_8H_{14} isomer	8.4
109	pentanoic acid	12	175	$C_{10}H_{10}$ isomer	4.8
111	2-methylpentanoic acid	3	177	unknown	NQ
112	$C_6H_{12}O$ isomer	2.4	178	C_9H_{16} + C_3-alkylpyridine isomer	T
116	$C_6H_{12}O_2$ (carboxylic acid)	1.8	181	acetophenone	T
118	$C_6H_{12}O_2$ (carboxylic acid)	2.0	182	$C_{11}H_{14}$ isomer	T
120	n-hexanoic acid	108	184	$C_{12}H_{16}$ isomer	T
121	cyclopentanone	12.6	185	d_5-nitrobenzene (e[illegible])	
123	methylcyclopentanone isomer	T	192	naphthalene	3
127	$C_7H_{14}O_2$ isomer	4.2	200	phenol	15400
129	$C_7H_{14}O_2$ isomer	3.6	203	aniline	45.6
134	n-heptanoic acid	125	205	dimethylphenol isomer	113
139	anisole	6.6	207	$C_6H_9O_2N$	T
141	$C_8H_{12}O_2$ (carboxylic acid)	T	211	isopropylphenol isomer	3
144	methylpyridine isomer	4.2	217	cresol isomer	3600
146	n-octanoic acid	148	222	C_3-alkyl phenol isomer	
147	C_7H_{12} isomer	T	223	C_2-alkyl phenol isomer	34
152	ethylphenol isomer	9	225	cresol isomer	16800
156	$C_7H_{14}O$ isomer (tent.)	NQ	226	dimethylphenol isomer	210
159	indene	T	227	cresol isomer	106
160	benzofuran	T	230	C_2-alkyl phenol isomer	93
172	$C_{10}H_{12}$ isomer	T	235	C_2-alkyl phenol isomer	19.2

[a] Acids and bases were determined as their methyl esters and pentafluoropropionyl amides, respectively. See Table 9 for complete listing of semi-volatile acid fraction.

Table D38. SEMI-VOLATILE ORGANICS IN PRODUCED WATER (-9L) FROM WELL 5-6 IN SITU COAL GASIFICATION (LERC, ERDA)

Elution Temperature (°C)	Compound[a]	ppb
100	methyl ethyl ketone	6.6
102	$C_5H_{10}O$ isomer	2.4
104	2-pentanone	220
106	toluene	576
108	n-hexanal	160
109	n-pentanoic acid	48
111	$C_5H_{10}O_2$ (carboxylic acid)	140
112	4-methyl-2-pentanone	36
112	benzoic acid	T
112	$C_6H_{12}O_2$ (carboxylic acid)	T
113	C_9H_{18} isomer	T
116	toluic acid isomer	490
117	toluic acid isomer	390
118	n-heptaldehyde	48
120	cyclopentanone	680
120	n-hexanoic acid	2680
122	C_2-alkyl benzene isomer	T
123	2-methylcyclopentanone	110
123	C_6H_{10} isomer	24
124	$C_{10}H_{20}$ isomer	T
126	$C_7H_{14}O_2$ (carboxylic acid)	T
126	C_3-alkyl benzene isomer	T
127	3-methylcyclopentanone	T
128	$C_6H_{12}O_2$ (carboxylic acid)	T
128	$C_6H_{10}O$ isomer	T
129	$C_{10}H_{22}$ isomer	12
130	n-octanal	36
131	C_3-alkyl benzene isomer	T
132	n-heptanoic acid	8870
137	dimethylpyridine isomer	580
138	3-methylpyridine isomer	250
139	4-methylpyridine isomer	100
139	anisole	230
140	2-n-propylpyridine	T
142	2,5-dimethyl-2-cyclopentenone	36
144	$C_6H_{10}O$ isomer	48
145	C_7H_{12} isomer	78
146	cyclohexenone or ethylcyclopentene isomer	T
146	C_5-alkyl benzene isomer	830
146	n-octanoic acid	1230
151	methylanisole isomer	36
159	indene	11
159	C_8H_{14} isomer (tent.)	T
160	benzofuran	T
169	unknown	NQ
171	$C_{10}H_{12}$ isomer	T
173	cyanobenzene	54
189	d_5-nitrobenzene (eS)	
193	C_3-alkyl phenol + C_2-alkyl phenol isomers	2560
197	cresol isomer	9
199	aniline	1290
205	ethylphenol isomer	42
214	phenol	22200
222	C_2-alkyl phenol isomer	4860
223	cresol isomer	10900
224	cresol isomer	4660

[a] Acids and bases were determined as their methyl esters and pentafluoropropionyl amides, respectively.

Table D39. SEMI-VOLATILE ORGANICS IN TAR (-10T) FROM WELL 5-6 IN SITU COAL GASIFICATION (LERC, ERDA)

Elution Temperature (°C)	Compound	ppm
92	CO_2	NQ
96	n-octane	40
98	ethyl formate	NQ
100	hydrocarbon	NQ
100	ethyl acetate	6800
100	n-nonane	2267
100	$C_{10}H_{22}$ isomer	1100
101	C_9H_{18} isomer	373
101	dimethyl ether	NQ
102	$C_{10}H_{22}$ isomer	100
103	$C_{10}H_{20}$ isomer	T
104	n-decane	3380
106	$C_{10}H_{20}$ isomer	113
107	toluene	2667
108	$C_{11}H_{24}$ isomer	T
110	$C_{10}H_{20}$ isomer	T
110	$C_{11}H_{22}$ + $C_{10}H_{18}$ isomers	73
112	n-undecane	3747
114	$C_{11}H_{22}$ isomer	280
115	ethylbenzene	87
116	$C_{11}H_{22}$ isomer	T
116	p-xylene	1400
117	m-xylene	1334
119	$C_{12}H_{24}$ isomer	T
120	C_3-alkyl benzene isomer	T
121	$C_{13}H_{28}$ isomer	T
122	n-dodecane + o-xylene	5040
125	n-propylbenzene	80
126	$C_{12}H_{24}$ isomer	T
127	ethyltoluene isomer	3747
128	$C_{13}H_{28}$ isomer	513
129	trimethylbenzene isomer	240
130	$C_{13}H_{28}$ isomer	T
130	dimethylpyridine isomer	973
131	styrene	T
131	methylpyridine isomer	47
132	C_3-alkyl benzene isomer	693
132	C_4-alkyl benzene isomer	513
133	$C_{13}H_{26}$ isomer	T
134	trimethylbenzene isomer + n-tridecane	5100
136	C_2-alkyl pyridine isomer	327
137	C_4-alkyl benzene isomer	34
137	C_3-alkyl pyridine isomer	T
138	$C_{13}H_{26}$ isomer	T
138	n-butylbenzene	113
139	$C_{14}H_{28}$ isomer	T
140	C_4-alkyl benzene isomer	T
140	$C_{13}H_{26}$ isomer	127
141	$C_{15}H_{30}$ isomer	T
142	trimethylbenzene isomer	2433
143	$C_{13}H_{26}$ isomer	413
144	C_4-alkyl benzene isomer	34
144	methylstyrene isomer	207
145	dimethylpyridine isomer	T
145	C_4-alkyl benzene isomer	180
146	C_9H_{10} isomer	T
147	n-tetradecane	1507
147	C_3-alkyl pyridine isomer	T
148	n-octanoic acid	34
149	C_5-alkyl benzene isomer	1140
149	n-nonanal	613
149	C_2-alkyl pyridine isomer	53
149	$C_{10}H_{12}$ isomer	113
150	C_5-alkyl benzene isomer	T
151	n-pentylbenzene	307
151	C_4-alkyl pyridine isomer	T
151	$C_{16}H_{34}$ isomer	20
152	C_4-alkyl pyridine isomer	T
153	$C_{14}H_{28}$ + C_5-alkyl benzene isomers	273
153	C_3-alkyl pyridine isomer	T
154	C_4-alkyl benzene + C_5-alkyl benzene isomers	20
154	C_5-alkyl pyridine isomer	T
154	dimethylethylpyridine isomer	7
155	C_4-alkyl benzene isomer	47
156	C_5-alkyl benzene isomer	T
157	C_6-alkyl benzene isomer	T
157	$C_{15}H_{30}$ isomer	173
159	$C_{15}H_{30}$ isomer	T
160	n-pentadecane + $C_{10}H_{12}$ isomer	74
162	indene	1467
162	C_4-alkyl benzene isomer	T
164	$C_{10}H_{12}$ + $C_{11}H_{14}$ isomers	1040
164	$C_{10}H_{12}$ isomer	1147
165	phenyl-n-hexane	143
166	$C_{15}H_{30}$ isomer	T
167	dimethylindan isomer	133
168	C_6-alkyl benzene isomer	75
169	$C_{15}H_{30}$ isomer	T
169	$C_7H_{10}O$ isomer	T

(continued)

Table D39 (cont'd)

Elution Temperature (°C)	Compound	ppm
170	$C_{15}H_{28}$ isomer	120
172	C_5-alkyl benzene isomer (tent.)	T
173	$C_{12}H_{16}$ isomer	T
175	*n*-hexadecane	1600
175	methylindene isomer	776
176	methylbenzofuran isomer	280
178	methylbenzofuran isomer	2907
178	methylindene isomer	
179	$C_{16}H_{32}$ isomer	
179	phenyl-*n*-heptane	193
180	$C_{12}H_{16}$ isomer	T
180	$C_{17}H_{36}$ isomer	7
181	$C_{11}H_{14}$ isomer	87
184	C_9-alkyl benzene isomer (tent.)	100
185	$C_{11}H_{14}$ isomer	107
187	dimethylbenzofuran isomer	20
188	$C_{12}H_{16}$ isomer	T
189	$C_{17}H_{36}$ + $C_{11}H_{12}$ isomers	147
189	$C_{13}H_{18}$ isomer	T
191	dimethylbenzofuran isomer	T
192	$C_{11}H_{12}$ isomer	127
193	$C_{19}H_{40}$ isomer	T
194	$C_{19}H_{38}$ isomer	53
195	d_5-nitrobenzene (e[illegible])	
196	naphthalene	13000
197	*n*-octadecane	207
199	$C_{14}H_{20}$ isomer	780
199	C_7H_9N isomer	280
200	$C_{19}H_{38}$ + $C_{12}H_{16}$ isomers	20
202	$C_{14}H_{20}$ isomer	T
203	2,3-benzothiophene	227
204	hydrocarbon	80
206	$C_{13}H_{18}$ isomer	113
207	$C_{18}H_{38}$ isomer	T
207	$C_8H_{11}N$ isomer	187
207	aniline	1400
209	methylnaphthalene isomer	6253
209	*n*-nonadecane	653
211	$C_{18}H_{36}$ isomer	780
212	C_7H_9N isomer	533
212	dimethylphenol isomer	1033
213	methylnaphthalene isomer	5720
215	C_7H_9N isomer	1267
216	pentamethylindane isomer	20
217	C_3-alkyl phenol isomer	78
219	$C_{15}H_{22}$ isomer	T
220	ethylnaphthalene isomer	367
220	C_2-alkyl naphthalene isomer	T
221	*n*-eicosane	93
221	quinoline	1087
222	dimethylnaphthalene isomer	4733
222	cresol isomer	9607
222	methylquinoline or $C_{10}H_9N$ isomer	113
223	phenol	1090
224	biphenyl	380
225	dimethylnaphthalene isomer	T
226	$C_{14}H_{10}$ isomer (tent.)	340
227	dimethylnaphthalene isomer	525
227	C_2-alkyl phenol isomer	370
229	C_2-alkyl phenol isomer (ethylphenol ?)	393
230	dimethylphenol isomer	4653
231	dimethylnaphthalene isomer	213
231	cresol isomer	10233
232	C_3-alkyl naphthalene isomer	T
232	*n*-heneicosane	587
232	cresol isomer	11680
234	C_2-alkyl naphthalene isomer	353
234	unknown	NQ
235	methylbiphenyl isomer	T
235	C_2-alkyl quinoline isomer (tent.)	100
236	C_3-alkyl phenol isomer	1400
236	C_3-alkyl naphthalene isomer	T
237	dimethylphenol isomer	334
238	trimethylnaphthalene isomer	T
238	C_3-alkyl phenol isomer	613
239	C_3-alkyl phenol isomer	340
240	tri-sec-butylphenol isomer	100
240	dimethylphenol isomer	720
240	biphenylacetylene or $C_{14}H_{10}$ isomer	153
240	C_3-alkyl naphthalene isomer	T
240	C_4-alkyl naphthalene isomer	T
240	acenaphthene	580
240	C_4-alkyl phenol isomer	T
240	C_3-alkyl phenol isomer	120

(continued)

Table D39 (cont'd)

Elution Temperature (°C)	Compound	ppm	Elution Temperature (°C)	Compound
240	C_3-alkyl naphthalene isomer	T		
	C_3-alkyl phenol isomer	805		
	C_3-alkyl naphthalene isomer	T		
	tri-butylphenol isomer	93		
	C_4-alkyl phenol isomer	T		
	biphenylene	T		
	C_3-alkyl phenol isomer	260		
	C_4-alkyl naphthalene isomer	T		
	C_5-alkyl naphthalene isomer	180		
	C_3-alkyl naphthalene isomer	35		
	C_4-alkyl phenol isomer	T		
	dibenzofuran	593		
	C_4-alkyl phenol isomer	27		
	C_4-alkyl phenol + alkyl naphthalene isomers	34		
	fluorene	293		
	C_3-alkyl phenol isomer	T		
	2,4,6-tri-sec-butylphenol	T		
	C_2-alkyl phenol isomer	8807		
	C_2-alkyl phenol isomer	4087		
	C_3-alkyl naphthalene isomer	107		
	C_3-alkyl phenol isomer	T		
	C_2-alkyl phenol isomer	390		
	tri-butylphenol isomer	3033		
	1,6-dimethyl-4-isopropylnaphthalene	T		
	C_3-alkyl phenol isomer	2806		
	C_3-alkyl phenol isomer	853		
	$C_{14}H_{10}$ isomer	T		
	hydroxyfluorene or dimethylbiphenyl isomer	T		
↓	dimethylphenanthrene	T		

Table D40. SEMI-VOLATILE ORGANICS IN PRODUCED WATER (-11L) FROM WELL 5-6 *IN SITU* COAL GASIFICATION (LERC, ERDA)

Elution Temp. (°C)	Compound	ppb
97	methyl ethyl ketone	246
99	benzene	3
100	2-pentanone	16
100	*n*-pentanal	T
100	methyl isopropyl ketone	246
101	*n*-butanoic acid	96
102	3-pentanone	T
102	isopentanoic acid	120
102	α-methylbutanoic acid	T
103	4-methyl-2-pentanone + isobutyronitrile	6
103	C_8H_{16} isomer	9
104	3-methyl-2-pentanone	1.2
105	toluene	150
105	propionitrile	T
106	3-hexanone	T
106	unknown	NQ
107	unknown	NQ
107	2-hexanone	9
107	*n*-pentanoic acid	840
108	2-methylpentanoic acid	35
109	α-methylbutyronitrile	T
110	*n*-butyronitrile	16
111	β-methylpentanoic acid	67
112	unknown	NQ
112	ethylbenzene	3
112	$C_7H_{14}O_2$ isomer	218
113	*p*-xylene	8.4
115	unknown	NQ
116	methylhexanal isomer	17
117	*n*-hexanoic acid	119
117	*n*-hexanal	T
118	*o*-xylene	15
119	cyclopentanone	T
119	C_2-alkyl thiophene isomer	T
119	*n*-pentylnitrile	462
120	2-pentylfuran (tent.)	T
120	methylcyclopentanone isomer	28
122	isopropylbenzene	T
123	$C_8H_{16}O_2$ isomer	23
123	methylcyclopentanone isomer	9
125	$C_8H_{16}O_2$ isomer	4.8
126	styrene	T
127	2-methylcyclobutane carboxylic acid	T
128	*n*-heptanoic acid	462
132	*n*-butylbenzene	9
136	anisole	126
148	methyl-*p*-cresyl ether	64
150	*n*-pentadecane	T
152	*n*-nonanal (tent.)	6
156	indene	99
158	pyrrole	213
158	benzofuran	T
183	$C_{17}H_{34}$ isomer	T
188	d_5-nitrobenzene (es)	
194	unknown	NQ
199	aniline	966
206	dimethylphenol isomer	471
208	dimethylphenol isomer	34
213	phenol + cresol isomer	saturated
221	ethylphenol isomer	
222	dimethylphenol isomer	
223	cresol isomer	
229	C_2-alkyl phenol isomer	
229	C_3-alkyl phenol isomer	
230	dimethylphenol isomer	
232	C_2-alkyl phenol isomer	
232	C_4-alkyl phenol isomer	
234	C_3-alkyl phenol isomer	
235	C_3-alkyl phenol isomer	
236	C_2-alkyl phenol isomer	
239	C_3-alkyl phenol iscmer	
240	C_3-alkyl phenol isomer	

Table D41. SEMI-VOLATILE ORGANICS IN PRODUCED TAR (-12T) FROM WELL 5-6 *IN SITU* COAL GASIFICATION (LERC, ERDA)

Elution Temperature (°C)	Compound	ppm	Elution Temperature (°C)	Compound	ppm
93	CO_2	NQ	142	C_4-alkyl benzene isomer	T
97	ethyl formate	NQ	143	$C_{15}H_{32}$ isomer	200
97	*n*-octane	800	144	C_2-alkyl pyridine isomer	T
99	ethyl acetate	NQ	144	C_4-alkyl benzene isomer	T
99	C_9H_{20} isomer	T	144	trimethylbenzene isomer	820
100	*n*-nonane	1520	145	C_2-alkyl pyridine isomer	740
102	$C_{10}H_{22}$ isomer	240	146	C_4-alkyl benzene isomer	T
102	dimethyl ether	NQ	146	methylstyrene or C_9H_{10} isomer	T
103	C_9H_{18} isomer	160	147	C_4-alkyl benzene isomer	T
103	$C_{10}H_{22}$ isomer	T	147	C_3-alkyl pyridine isomer	T
105	*n*-decane	3520	148	C_4-alkyl benzene isomer	T
108	$C_{10}H_{20}$ isomer	280	149	indan + *n*-tetradecane	1180
109	toluene	840	149	C_4-alkyl pyridine isomer	1020
110	$C_{10}H_{28}$ + $C_{11}H_{22}$ isomers	T	151	C_4-alkyl benzene isomer	540
110	$C_{11}H_{24}$ isomer	T	152	C_5-alkyl benzene isomer	500
111	$C_6H_{12}O$ isomer	T	153	methylindan isomer	T
113	*n*-undecane	2080	154	$C_{16}H_{34}$ isomer + *n*-pentylbenzene	300
116	$C_{11}H_{22}$ isomer	1160			
116	ethylbenzene	300	155	$C_{14}H_{28}$ isomer	T
117	xylene isomer	T	156	$C_{15}H_{30}$ + C_4-alkyl benzene isomers	T
118	xylene isomer	1660			
119	$C_{12}H_{26}$ isomer	420	157	C_5-alkyl benzene isomer	20
119	xylene isomer	820	158	C_4-alkyl benzene isomer	40
120	$C_{11}H_{22}$ isomer	T	159	C_5-alkyl benzene isomer	T
121	$C_{12}H_{26}$ isomer	T	160	C_6-alkyl benzene + $C_{14}H_{28}$ isomers	30
123	isopropylbenzene	T			
123	$C_{13}H_{28}$ isomer	T	161	C_6-alkyl benzene isomer	T
124	*n*-dodecane	3700	162	*n*-pentadecane	1240
127	*n*-propylbenzene	60	163	methylindan isomer	300
128	$C_{12}H_{24}$ isomer	T	164	indene	1580
129	ethyltoluene isomer	1540	164	C_4-alkyl benzene isomer	T
129	C_2-alkyl pyridine isomer	580	165	C_2-alkyl indan isomer	T
130	$C_{13}H_{28}$ isomer	T	166	benzofuran	780
130	methylpyridine isomer	T	166	$C_{10}H_{12}$ isomer	T
131	trimethylbenzene isomer	260	167	$C_{11}H_{14}$ isomer	T
132	$C_{12}H_{24}$ isomer	T	168	$C_{15}H_{30}$ isomer	T
133	styrene	T	169	C_2-alkyl indan isomer	40
134	ethyltoluene isomer	340	170	$C_{15}H_{30}$ isomer	T
135	C_4-alkyl benzene isomer	T	172	$C_{15}H_{28}$ isomer	120
136	C_4-alkyl pyridine isomer	440	175	$C_{11}H_{14}$ isomer	T
136	*n*-tridecane	2300	176	*n*-hexadecane	40
136	trimethylbenzene isomers	1240	178	methylindene isomer	260
139	C_4-alkyl benzene isomer	T	178	methylbenzofuran isomer	T
140	$C_{13}H_{26}$ isomer	T	180	methylbenzofuran isomer	660
140	*n*-butylbenzene	T	180	methylindene isomer	280
141	$C_{14}H_{28}$ isomer	T	181	$C_{12}H_{16}$ isomer	T

(continued)

Table D41 (cont'd)

Elution Temperature (°C)	Compound	ppm
182	trimethylindan isomer	T
183	C_2-alkyl indan isomer	T
184	$C_{16}H_{32}$ isomer	20
186	C_9-alkyl benzene + $C_{17}H_{36}$ isomers	80
190	$C_{12}H_{16}$ isomer	T
190	$C_{17}H_{34}$ isomer	T
191	*n*-heptadecane	40
192	dimethylbenzofuran isomer	20
193	$C_{13}H_{18}$ isomer	T
193	$C_{11}H_{12}$ isomer	T
195	phenyl-*n*-octane (tent.)	T
195	$C_{11}H_{12}$ isomer	50
196	$C_{17}H_{34}$ isomer	T
197	d_5-nitrobenzene (eB)	
197	*n*-octadecane	320
197	naphthalene	16400
197	C_7H_9N isomer	60
201	$C_{12}H_{16}$ isomer	60
201	$C_8H_{11}N$ isomer	250
203	aniline	1380
203	$C_{12}H_{16}$ isomer	T
205	2,3-benzothiophene	80
207	*n*-nonadecane	1540
207	$C_{13}H_{18}$ isomer	T
209	$C_{14}H_{20}$ isomer	T
209	$C_{19}H_{40}$ isomer	520
209	C_7H_9N isomer	260
211	methylnaphthalene isomer	5100
212	benzylamine	60
215	phenol	580
215	dimethylphenol isomer	T
215	$C_8H_{11}N$ isomer	T
215	cresol isomer	12180
215	methylnaphthalene isomer	2860
217	pentamethylindan isomer	60
217	quinoline	140
218	*n*-eicosane	2200
219	C_3-alkyl phenol isomer	80
219	methylquinoline isomer	340
221	ethylnaphthalene isomer	120
222	$C_{20}H_{42}$ isomer	700
223	C_2-alkyl naphthalene isomer	1280
223	dimethylnaphthalene isomer	T
224	C_3-alkyl phenol isomer	T
225	biphenyl	60
225	methylquinoline isomer (tent.)	T
226	C_3-alkyl phenol isomer	T
228	dimethylnaphthalene isomer	4000
228	cresol isomer	340
229	ethylphenol isomer	100
229	*n*-heneicosane	1140
230	ethylphenol isomer	T
231	dimethylphenol isomer	3520
231	cresol isomer	16860
231	C_2-alkyl quinoline isomer (tent.)	T
232	C_4-alkyl phenol isomer	T
232	C_3-alkyl phenol isomer	T
233	C_3-alkyl naphthalene isomers	140
233	C_2-alkyl phenol isomer	T
234	C_3-alkyl naphthalene isomer	100
234	C_3-alkyl phenol isomer	T
235	dimethylnaphthalene isomer	T
236	$C_{14}H_{10}$ isomer	T
236	C_3-alkyl phenol isomer	120
236	di-sec-butylphenol isomer + unknown	3440
237	C_3-alkyl phenol isomer	140
237	dimethylphenol isomer	160
238	C_3-alkyl naphthalene isomer	T
238	ethylphenol isomer (tent.)	T
240	C_3-alkyl naphthalene isomer	T
240	*n*-$C_{22}H_{46}$ isomer	60
240	C_3-alkyl phenol + tri-sec-butylphenol (tent.)	1160
240	dimethylphenol isomer	T
240	acenaphthene	820
240	C_3-alkyl phenol isomer	T
240	C_3-alkyl naphthalene isomer	T
240	C_3-alkyl phenol isomer	7300
240	tri-butylphenol isomer	4760
240	biphenylene	T
240	C_3-alkyl phenol isomer	T
240	C_5-alkyl naphthalene isomer	T
240	C_3-alkyl phenol isomer	T
240	C_5-alkyl naphthalene isomer	T
240	C_4-alkyl phenol + C_3-alkyl naphthalene isomers (tent.)	140

(continued)

Table D41 (cont'd)

Elution Temperature (°C)	Compound	ppm	Elution Temperature (°C)	Compound
240	C_4-alkyl phenol isomer (tent.)	T		
240	fluorene	140		
240	methylphenanthrene isomer	T		
240	dimethylisopropylnaphthalene isomer (tent.)	T		

Table D42. SEMI-VOLATILE ORGANICS IN PRODUCED WATER (-13L) FROM WELL 5-6 *IN SITU* COAL GASIFICATION (LERC, ERDA)

Elution Temp. (°C)	Compound	ppb
97	C_5H_{12} isomer	NQ
98	methyl ethyl ketone	NQ
99	methyl isopropyl ketone	NQ
99	propanal	NQ
100	benzene	156
101	*n*-butanal	NQ
101	2-pentanone	1170
101	*n*-butyric acid	90
102	4-methyl-2-pentanone	80
103	isopentanoic acid	170
103	3-methyl-2-pentanone	110
104	*n*-propionitrile (tent.)	130
104	$C_5H_{10}O_2$ carboxylic acid	42
105	toluene	90
105	3-hexanone	T
106	$C_5H_{10}O_2$ carboxylic acid	T
106	2-methyl-1,3-dioxane	T
107	2-hexanone	140
107	*n*-pentanoic acid	1060
107	2-methylpentanoic acid	260
108	α-methylbutyronitrile	T
109	*n*-butyronitrile	84
110	$C_7H_{14}O$ isomer	T
111	ethylbenzene	T
112	*p*-xylene	140
112	isohexanoic acid	190
113	C_2-alkyl benzene isomer	T
114	unknown	NQ
116	*n*-hexanoic acid	1470
117	*o*-xylene	66
118	*n*-pentylnitrile	T
119	cyclopentanone	48
119	methylcyclopentanone + *n*-propylbenzene	T
120	$C_8H_{16}O_2$ carboxylic acid	T
121	2-*n*-pentylfuran	T
122	$C_6H_{10}O$ isomer	48
123	$C_8H_{16}O_2$ carboxylic acid	78
124	isoheptanoic acid	30
128	*n*-heptanoic acid	870
132	*n*-butylbenzene	18
136	anisole	100
141	*n*-octanoic acid	110
145	*n*-pentylbenzene	T
149	*p*-cresyl methyl ether	18
153	dimethylpyridine + methylethylpyridine isomers	12
156	$C_{10}H_{12}$ isomer	T
156	indene	96
157	pyrrole	270
158	benzofuran	90
189	d_5-nitrobenzene (e[illegible])	
201	aniline	3460
204	dimethylphenol isomer	990
215	phenol + cresol isomer	270000
217	dimethylphenol isomer	600
220	ethylphenol isomer	18
221	dimethylphenol isomer	60
222	cresol isomer	850
223	cresol isomer	10200
227	C_3-alkyl phenol isomer	170
227	C_3-alkyl phenol isomer	180
229	C_3-alkyl phenol isomer	830
231	dimethylphenol isomer	7800
235	C_3-alkyl phenol isomer	6
237	C_2-alkyl phenol isomer	8100

Table D43. SEMI-VOLATILE ORGANICS IN PRODUCED WATER (-14L) FROM WELL 7-8 IN SITU COAL GASIFICATION (LERC, ERDA)

Chromato-graphic Peak No.	Elution Temp. (°C)	Compound	ppm
	99	benzene	11
	99	n-butyric acid	4.2
	101	n-pentanal	6
	102	$C_{10}H_{22}$ isomer	T
	102	$C_5H_{10}O_2$ isomer	8.4
	103	α-methylbutyric acid (tent.)	9
	104	$C_5H_{10}O_2$ isomer	10
	105	toluene	3
	105	$C_5H_{10}O_2$ isomer	T
	107	n-hexanal	T
	107	acid (?)	T
	108	$C_5H_8O_2$ isomer	259
	108	$C_6H_{12}O_2$ isomer	226
	109	$C_{11}H_{24}$ isomer	T
	110	$C_6H_{12}O_2$ isomer	124
	111	$C_6H_{10}O_2$ isomer	35
	112	$C_6H_{12}O_2$ isomer	53
	113	C_2-alkyl benzene isomer	T
	114	$C_7H_{14}O_2$ acid	92
	114	3-heptanone	T
	116	α-C_2-alkyl $C_7H_{14}O_2$ acid	1.2
	117	2-heptanone	1.8
	117	n-heptanal	T
	119	$C_7H_{14}O_2$ carboxylic acid	514
	119	cyclopentanone	56
	120	2-methylcyclopentanone	58
	121	alkyl cyclohexane isomer	T
	122	3-methylcyclopentanone	37
	122	C_9H_{20} isomer	T
	123	C_2-alkyl cyclopentanone isomer (tent.)	T
	123	C_9H_{20} isomer	4.8
	124	C_3-alkyl benzene isomer (tent.)	T
	124	C_9H_{20} isomer	4.2
	125	styrene	T
	128	C_3-alkyl benzene isomer	T
	129	C_3-alkyl benzene isomer + 2-octanone	1.2
	130	2-ethyl cyclopentanone	5.4
	130	$C_7H_{14}O_2$ acid	244
	132	cyclohexanone	T
	132	n-butylbenzene or C_4-alkyl benzene isomer	T
	133	$C_7H_{12}O$ isomer	9
	136	C_3-alkyl benzene isomer	1.8
	137	2,5-dimethyl-2-cyclopentenone	T
	137	anisole	35
	139	dimethylcyclopentenone isomer	T
	139	diisopropylbenzene isomer	T
	140	indan	T
	141	$C_7H_{14}O_2$ carboxylic acid	T
	141	cyclohexenone isomer (tent.)	16
	145	phenyl-n-pentane	T
	145	C_2-alkyl phenol isomer	1.2
	146	$C_9H_{14}O$ isomer (tent.)	T
	149	$C_7H_{12}O_2$ + C_4-alkyl benzene isomers	0.6
	149	C_2-alkyl phenol isomer	19
	150	1-methyl-cyclohex-1-en-3-one (tent.)	T
	150	C_2-alkyl phenol	23
	151	$C_7H_{10}O$ isomer	T
	154	$C_{10}H_{12}$ isomer	T
	155	indene	7.2
	156	C_8H_{14} isomer (tent.)	T
	157	benzofuran	T
	158	$C_8H_{12}O$ isomer	14
	160	$C_9H_{14}O$ isomer	8.4
	164	$C_7H_{10}O$ isomer	172
	167	$C_8H_{12}O$ isomer	T
	168	methylindene isomer	T
	169	2-methylbenzofuran	3.6
	171	cyanobenzene	8.4
	172	methylindene	T
	177	acetophenone	9.8
	177	benzylcyanide or o-tolunitrile	2.4
	180	dimethylbenzofuran isomer	T
	180	methylacetophenone isomer	T
	182	$C_{10}H_{10}O$ isomer (tent.)	T
	183	methylcyanobenzene isomer	T
	188	d_5-nitrobenzene (e#)	
	189	naphthalene	242
	195	2,3-benzothiophene	1.2
	202	methylnaphthalene isomer	10
	205	dimethylphenol isomer	175
	207	methylnaphthalene isomer	6
	209	C_3-alkyl phenol isomer	55
	214	cresol isomer	503
	215	C_3-alkyl phenol isomer + phenol	2737
	220	C_3-alkyl phenol	11
	221	ethylphenol isomer	129
	223	dimethylphenol isomer	533
	224	cresol isomer	402

Table D44. SEMI-VOLATILE ORGANICS IN PRODUCED TAR (-15T) FROM WELL 7-8 IN SITU COAL GASIFICATION (LERC, ERDA)

Elution Temperature (°C)	Compound	ppm
92	CO_2	-
97	n-octane	20
97	acetone	NQ
99	n-butanal	NQ
100	n-nonane	50
101	$C_{10}H_{22}$ isomer	T
102	$C_{10}H_{20}$ isomer	T
103	$C_{10}H_{22}$ isomer	T
104	toluene	T
104	n-pentanal	80
104	C_9H_{18} isomer	70
105	n-decane	2500
107	$C_{10}H_{20}$ isomer	20
108	$C_6H_{12}O$ isomer	1340
109	toluene	1140
111	n-hexanal	40
122	$C_{11}H_{22}$ isomer	T
133	n-undecane	420
115	$C_{11}H_{22}$ isomer	T
116	ethylbenzene	320
117	$C_{11}H_{22}$ isomer	220
117	xylene isomer	280
119	xylene isomer	1540
120	$C_{12}H_{24}$ isomer	86
120	$C_{12}H_{26}$ isomer	T
122	isopropylbenzene + $C_{12}H_{24}$ isomer	T
122	n-heptanal	280
123	n-dodecane	220
124	xylene isomer	840
126	$C_{12}H_{24}$ isomer	46
126	n-propylbenzene	62
127	$C_{12}H_{24}$ isomer	T
128	ethyltoluene isomer	2200
130	$C_{13}H_{26}$ isomer	2500
131	trimethylbenzene isomer	260
132	styrene	80
133	C_3-alkyl benzene isomer	T
134	C_4-alkyl benzene isomer	440
135	n-tridecane	280
135	n-octanal	1140
136	trimethylbenzene isomer	4500
137	$C_{13}H_{26}$ isomer	T
137	C_6H_7N isomer	40
138	C_4-alkyl benzene isomer	20
139	n-butylbenzene	24
139	$C_8H_{11}N$	
140	$C_{13}H_{26}$ isomer	28
141	C_4-alkyl benzene + $C_{14}H_{28}$ isomers	38
141	$C_{14}H_{30}$ isomer	400
142	$C_{15}H_{32}$ isomer	520
143	C_4-alkyl benzene + $C_{14}H_{30}$ isomers	640
143	trimethylbenzene isomer	250
144	$C_{14}H_{30}$ isomer	280
145	methylstyrene + C_5-alkyl benzene isomers	54
146	C_4-alkyl benzene isomer	62
146	C_6H_7N isomer	T
147	C_4-alkyl benzene isomer	T
148	indan	3740
148	n-tetradecane	3540
149	$C_{10}H_{12}$ isomer	1120
149	n-nonanal	820
150	C_5-alkyl benzene isomer	540
151	methylindan	60
151	C_5-alkyl benzene + $C_{14}H_{28}$ isomers	40
151	$C_8H_{11}N$ isomer	740
152	$C_{16}H_{34}$ isomer	280
152	n-pentylbenzene	340
153	$C_{16}H_{34}$ isomer	220
154	$C_{14}H_{28}$ isomer	200
154	$C_{15}H_{30}$ isomer	194
155	C_5-alkyl benzene isomer	246
156	C_4-alkyl benzene isomer	234
157	C_5-alkyl benzene isomer	198
158	C_6-alkyl benzene + $C_{15}H_{30}$ isomers	94
160	$C_{15}H_{30}$ isomers	T
162	n-pentadecane + methylindan isomer	3540
163	indene	2540
163	C_4-alkyl benzene isomer	4420
163	n-decanal	440
164	C_4-alkyl benzene isomer	640
165	benzofuran	2300
165	$C_{10}H_{15}N$ isomer	94
166	$C_{11}H_{14}$ isomer	T
166	phenyl-n-hexane	20
167	$C_{15}H_{30}$ isomer	36

(continued)

Table D44 (cont'd)

Elution Temperature (°C)	Compound	ppm
168	dimethylindan isomer	350
169	C_6-alkyl benzene isomer	324
170	$C_{15}H_{30}$ isomer	T
171	$C_{15}H_{28}$ isomer	620
174	$C_{11}H_{18}$ isomer	80
175	$C_{12}H_{16}$ isomer	T
175	$C_{16}H_{32}$ isomer	T
176	n-hexadecane	920
177	methylindene isomer	780
179	methylbenzofuran isomer	720
179	methylindene + $C_{12}H_{16}$ isomer	880
181	$C_{12}H_{16}$ isomer	38
182	aldehyde (?)	NQ
182	$C_{16}H_{32}$ isomer	T
183	$C_{11}H_{14}$ isomer	354
184	$C_{12}H_{16}$ isomer	T
185	$C_{17}H_{36}$ isomer	T
186	C_9-alkyl benzene isomer	330
187	$C_{11}H_{14}$ isomer	308
187	$C_{12}H_{16}$ isomer	224
188	$C_{11}H_{14}$ isomer	160
189	trimethylindan isomer	42
190	$C_{11}H_{12}$ isomer	64
190	dimethylbenzofuran + alkylindan isomers	272
191	dimethylbenzofuran isomer	590
192	$C_{17}H_{36}$ isomer	632
192	alkyl indan isomer	560
193	$C_{11}H_{12}$ isomer	T
194	n-heptadecane + phenyl octane	280
195	d_5-nitrobenzene (eI)	
195	naphthalene	14440
195	n-octadecane	T
197	allylic acid	T
199	methylaniline	T
202	$C_{12}H_{16}$ isomer	66
203	alkyl indan isomer	T
204	2,3-benzothiophene	160
204	C_2-alkyl aniline	54
206	$C_{15}H_{22}$ isomer	20
206	aniline	2580
207	n-nonadecane	940
209	$C_{14}H_{20}$ isomer	80
210	methylnaphthalene isomer	11780
210	dimethylphenol isomer	840
212	benzylamine or methylaniline	820
213	dimethylphenol isomer	T
213	$C_{18}H_{36}$ isomer (tent.)	840
214	methylnaphthalene isomer	5120
215	C_3-alkyl phenol isomer	T
215	methylaniline isomer	2120
216	pentamethylindan isomer	38
218	C_3-alkyl phenol isomer	T
219	$C_{18}H_{36}$ isomer	100
219	cresol isomer	17000
219	C_2-alkyl aniline isomer	T
219	phenol	4500
220	ethylnaphthalene isomer	3400
220	C_2-alkyl aniline isomer	T
221	n-eicosane + quinoline	3100
222	cresol isomer	T
222	methylquinoline + cresol isomer	3000
222	dimethylnaphthalene isomer	940
223	C_3-alkyl phenol isomer	220
223	$C_{20}H_{40}$ isomer	780
224	biphenyl	680
225	dimethylnaphthalene isomer	6420
226	dimethylnaphthalene isomer	2900
226	ethylphenol isomer	T
226	C_2-alkyl aniline isomer	24200
227	dimethylphenol isomer	T
228	C_3-alkyl phenol isomer	T
229	ethylphenol isomer	22140
229	cresol isomer	T
229	C_2-alkyl naphthalene isomer	5540
230	dimethylphenol isomer	840
231	dimethylnaphthalene isomer	1520
232	cresol isomer	280
233	C_3-alkyl naphthalene + $C_{21}H_{44}$	200
233	n-heneicosane	260
233	C_3-alkyl phenol isomer	580
234	dimethylnaphthalene isomer	280
235	methylbiphenyl + $C_{15}H_{22}$ isomers	960
235	dimethylphenol isomer	60
235	C_3-alkyl quinoline isomer	640
236	C_3-alkyl phenol + C_3-alkyl naphthalene isomers	640
236	C_3-alkyl phenol isomers	940
237	C_2-alkyl phenol isomers	14500
238	ethylphenol isomer	280
238	C_2-alkyl phenol isomer	13720

(continued)

Table D44 (cont'd)

Elution Temperature (°C)	Compound	ppm	Elution Temperature (°C)	Compound
238	C_3-alkyl naphthalene isomer	80		
239	C_3-alkyl phenol isomer	300		
240	C_2-alkyl phenol + C_3-alkyl naphthalene isomers	4760		
240	C_4-alkyl naphthalene isomers	T		
240	acenaphthene	2040		
240	C_4-alkyl phenol isomer	T		
240	C_3-alkyl phenol isomer	T		
240	C_3-alkyl naphthalene isomer	T		
240	C_3-alkyl phenol + C_3-alkyl naphthalene isomers	580		
240	C_4-alkyl phenol isomer	T		
240	biphenylene	160		
240	sec-butylphenol isomer	T		
240	C_4-alkyl naphthalene isomer	T		
240	C_3-alkyl phenol isomer	3169		
240	C_3-alkyl phenol isomer	3440		
240	C_3-alkyl naphthalene isomer	T		
240	C_4-alkyl phenol isomer	T		
240	C_5-alkyl naphthalene isomer	T		
240	dibenzofuran	640		
240	fluorene	580		
240	$C_{13}H_{10}O$ or $C_{14}H_{14}$ isomer	T		
240	tri-sec-butylphenol isomer	3840		
240	dimethylbenzaldehyde isomer	560		
240	dimethylbenzaldehyde isomer	640		
240	C_3-alkyl benzaldehyde isomer (tent.)	100		

Table D45. SEMI-VOLATILE ORGANICS IN PRODUCED WATER (-16L) FROM WELL 7-8 IN SITU COAL GASIFICATION (LERC, ERDA)

Elution Temp. (°C)	Compound	ppb
97	methyl ethyl ketone	NQ
98	methyl isopropyl ketone	NQ
99	benzene	T
99	3-pentanone (tent.)	T
100	2-pentanone	700
101	butanoic acid	75
101	4-methyl-2-pentanone	T
102	3-methyl-2-pentanone	105
102	α-methylbutanoic acid	T
103	isopentanoic acid	400
103	toluene	150
103	3-hexanone	60
105	2-hexanone	275
107	$C_{10}H_{20}$ isomer	T
107	α-methylbutyronitrile + 4,4-dimethyl-2-pentanone (tent.)	T
107	n-butyronitrile	30
108	ethanol (tent.)	T
108	$C_7H_{14}O$ isomer	T
108	pentanoic acid	4825
109	$C_7H_{14}O$ isomer	60
110	2-methylpentanoic acid	1150
110	ethylbenzene	T
111	p-xylene	45
112	5-methyl-3-hexanone	15
114	β-methylpentanoic acid	725
115	2-heptanone + o-xylene	225
116	cyclopentanone	3400
117	2-methylcyclopentanone	2075
119	n-hexanoic acid	5950
120	3-methylcyclopentanone	2100
121	C_2-alkyl cyclopentanone isomer (tent.)	650
123	$C_{10}H_{16}$ isomer	425
124	C_3-alkyl benzene isomer	T
127	$C_7H_{12}O$ + C_3-alkyl benzene isomers	180
129	n-hexylnitrile	250
129	$C_7H_{12}O$ isomer	T
131	cyclohexanone	210
134	heptanoic acid	1925
134	C_3-alkyl benzene isomer	180
136	anisole	1075
139	o-methylstyrene or indan	135
142	$C_7H_{10}O$ isomer	T
146	$C_7H_{10}O$ isomer	T
150	methylanisole isomer (tent.)	T
152	$C_9H_{18}O_2$ carboxylic acid	NQ
152	C_6H_8O isomer	925
154	indene	275
156	benzofuran	120
158	$C_{13}H_{26}$ isomer	75
160	$C_8H_{10}S$ isomer (tent.)	60
164	dimethylfuran isomer (tent.)	T
164	benzaldehyde	T
165	dimethylcyclopentenone	375
166	decanoic acid	1600
166	diethylfuran isomer	T
170	C_9H_8O isomer	T
171	cyanobenzene	1350
172	methylindene isomer (tent.)	90
175	$C_{17}H_{36}$ isomer	T
184	unknown	NQ
186	unknown	NQ
188	m-methylbenzoic acid	T
189	d_5-nitrobenzene (es)	
190	naphthalene	3075
190	C_5-alkyl benzene isomer	60
190	dimethylphenol isomer	T
190	dimethylbenzoic acid isomer	T
191	unknown	NQ
191	dimethylbenzoic acid isomer	T
192	C_3-alkyl benzoic acid isomer	T
194	dimethylphenol isomer	250
194	dimethylbenzoic acid isomer	325
195	C_5-alkyl benzene isomer	450
197	benzothiophene	200
204	dimethylphenol isomer	5650
205	methylaniline isomer	1325
207	methylaniline isomer	1150
210	C_3-alkyl phenol isomer	250
211	dimethylaniline isomer	T
212	dimethylaniline isomer	T
213	cresol isomer	225000
214	phenol	
218	cyclopentenol isomer	T
220	trimethylphenol isomer	180
221	dimethylphenol isomer	45
223	dimethylphenol isomer	210
223	C_3-alkyl phenol isomer	250

(continued)

Table D45 (cont'd)

Elution Temp. (°C)	Compound	ppb	Elution Temp. (°C)	Compound
224	butylanisole isomer	90		
227	methylethylphenol isomer	3625		
227	cresol isomer	2675		
228	cresol isomer	T		
228	C_2-alkyl phenol isomer	75		
229	C_3-alkyl phenol isomer	3200		
231	C_2-alkyl phenol isomer	2200		
231	C_2-alkyl phenol isomer	2600		
232	ethylphenol isomer	400		
232	C_4-alkyl phenol isomer	296725		
232	C_3-alkyl phenol isomer			
233	C_3-alkyl phenol isomer			
235	C_3-alkyl phenol isomer			
237	C_4-alkyl phenol isomer			
240	C_3-alkyl phenol isomer			
240	C_3-alkyl phenol isomer			
240	C_3-alkyl phenol isomer			
240	C_4-alkyl phenol isomer			
240	unsaturated C_4-alkyl phenol isomer	T		
240	indole (tent.)	275		

Table D46. SEMI-VOLATILE ORGANICS IN PRODUCED TAR (-17T) FROM WELL 7-8 *IN SITU* COAL GASIFICATION (LERC, ERDA)

Elution Temperature (°C)	Compound	ppm[a]	Elution Temperature (°C)	Compound	ppm
92	CO_2	-	138	C_4-alkyl benzene isomer	120
95	acetaldehyde	NQ	140	*n*-butylbenzene + $C_{13}H_{26}$ isomer	40
96	acetone	NQ	140	C_3-alkyl phenol isomer (?)	NQ
97	*n*-octane	40	141	$C_{14}H_{28}$ isomer	80
97	ethyl formate	NQ	141	C_4-alkyl benzene isomer	T
99	C_9H_{20} isomer	1100	142	C_4-alkyl benzene + $C_{13}H_{26}$ isomers	260
99	ethyl acetate	NQ	143	$C_{15}H_{32}$ isomer	240
99	*n*-butanal	NQ	143	$C_9H_{13}N$ isomer	40
100	*n*-nonane	680	144	trimethylbenzene isomer	1320
101	dimethyl ether	NQ	145	C_4-alkyl benzene isomer	260
102	$C_{10}H_{22}$ isomer	420	146	methylstyrene + C_5-alkyl benzene isomers	280
103	C_9H_{18} isomer	380	146	C_4-alkyl benzene isomer	180
104	C_9H_{18} isomer	T	147	C_4-alkyl benzene isomer	40
104	$C_5H_{10}O$ isomer	T	149	indan	2080
105	*n*-decane	1840	150	*n*-tetradecane	1720
108	$C_{10}H_{20}$ isomer	280	150	$C_{10}H_{12}$ isomer	280
108	$C_{11}H_{24}$ isomer	640	151	C_5-alkyl benzene isomer	60
109	toluene	820	152	methylindan isomer	40
110	$C_{11}H_{24}$ isomer	120	153	C_5-alkyl benzene + $C_{14}H_{28}$ isomers	20
111	$C_5H_{10}O$ (ketone ?)	T	153	*n*-pentylbenzene	120
112	$C_{11}H_{22}$ isomer	T	154	$C_{16}H_{34}$ isomer	100
114	*n*-undecane	1940	155	$C_{14}H_{28}$ isomer	440
116	ethylbenzene	320	157	C_5-alkyl benzene isomur	160
117	xylene isomer	260	157	C_4-alkyl benzene isomer	80
117	$C_{11}H_{22}$ isomer	160	158	C_5-alkyl benzene isomer	60
118	xylene isomer	1760	159	C_6-alkyl benzene isomer	40
120	$C_{12}H_{26}$ isomer	140	159	$C_{15}H_{30}$ isomer	160
121	C_3-alkyl benzene + $C_{11}H_{22}$ isomers	60	162	methylindan isomer	180
122	$C_7H_{14}O$ isomer	T	163	*n*-$C_{15}H_{32}$ isomer	860
123	xylene isomer	1120	164	indene	2280
124	*n*-dodecane	2220	165	benzofuran	1540
127	*n*-propylbenzene	40	166	dimethylindan isomer	1160
127	C_2-alkyl phenol isomer (?)	NQ	166	$C_{10}H_{12}$ isomer	1780
128	$C_{12}H_{24}$ isomer	T	167	phenyl-*n*-hexane	1100
129	ethyltoluene isomer	1240	167	$C_{15}H_{30}$ isomer	500
130	$C_{12}H_{24}$ isomer	1720	168	$C_{11}H_{14}$ isomer	760
131	trimethylbenzene isomer	180	169	dimethylindan isomer	900
133	styrene	80	170	$C_{15}H_{30}$ + C_6-alkyl benzene isomers	340
133	ethyltoluene isomer	300	171	$C_7H_{10}O$ isomer (tent.)	140
133	C_7H_9N isomer	T	172	$C_{15}H_{28}$ isomer	120
134	C_4-alkyl benzene isomer	140	174	C_5-alkyl benzene isomer	80
134	C_6H_7N isomer	T	175	$C_{11}H_{14}$ isomer	60
135	$C_{13}H_{28}$ isomer	120			
136	trimethylbenzene isomer + *n*-tridecane	2540			

(continued)

Table D46 (cont'd)

Elution Temperature (°C)	Compound	ppm
176	$C_{11}H_{14}$ isomer	100
177	methylindene isomer + n-hexadecane	40
178	methylbenzofuran isomer	300
179	methylbenzofuran isomer (tent.)	1300
180	methylindene isomer (tent.)	280
181	$C_{16}H_{34}$ isomer	1660
182	n-hexadecane	80
185	$C_{16}H_{32}$ isomer	T
186	C_9-alkyl benzene isomer	60
186	n-heptadecane	100
187	$C_{13}H_{18}$ isomer	20
187	$C_{12}H_{16}$ isomer	T
189	dimethylbenzofuran isomer	T
189	$C_{12}H_{16}$ isomer	T
190	$C_{11}H_{12}$ isomer	T
191	dimethylbenzofuran isomer (tent.) + alkylindan isomer	340
192	dimethylbenzofuran isomer	380
192	$C_{17}H_{36}$ isomer	500
193	$C_{11}H_{12}$ isomer	540
194	n-$C_{17}H_{36}$ isomer	T
194	$C_{19}H_{38}$ isomer	T
194	$C_{19}H_{38}$ isomer	T
195	phenyl-n-octane + methyl dihydronaphthalene isomer	340
196	d_5-nitrobenzene (es)	
196	naphthalene	930
198	n-$C_{18}H_{38}$ isomer	440
199	$C_{18}H_{36}$ isomer	300
199	$C_{14}H_{20}$ isomer (tent.)	280
201	methylaniline	80
201	C_3-alkyl benzofuran (tent.)	40
202	$C_{12}H_{16}$ isomer	60
204	2,3-benzothiophene	80
205	hydrocarbon (?) + unknown	T
207	$C_{13}H_{13}$ isomer	60
207	$C_{19}H_{40}$ isomer	40
208	$C_{14}H_{20}$ isomer	T
208	aniline + methylnaphthalene isomer	60
208	$C_{14}H_{20}$ isomer	T
209	methylnaphthalene isomer	630
210	n-$C_{19}H_{40}$ isomer	3100
213	dimethylnaphthalene isomer	T
213	dimethylphenol isomer	NQ
214	$C_{14}H_{20}$ isomer	T
214	benzylamine + dimethylnaphthalene + quinoline	80
215	dimethylnaphthalene isomer	2880
216	$C_{19}H_{38}$ isomer	40
217	pentamethylindan isomer	100
218	$C_{20}H_{40}$ isomer	80
218	C_3-alkyl phenol isomer	NQ
219	C_2-alkyl naphthalene isomer (tent.)	T
221	ethylnaphthalene isomer	440
221	cresol isomer + phenol	45000
222	n-$C_{20}H_{42}$ isomer	1960
223	dimethylnaphthalene isomer	2140
223	C_2-alkyl naphthalene isomer	780
223	C_3-alkyl phenol isomer	1540
224	cresol isomer	2720
225	biphenyl	640
226	dimethylnaphthalene isomer	780
227	dimethylnaphthalene isomer + $C_{20}H_{40}$ isomers	3140
229	dimethylphenol isomer	NQ
229	ethylphenol	540
230	dimethylphenol isomer	3240
230	cresol isomer	55000
231	dimethylnaphthalene	2500
231	cresol isomer	79520
232	C_2-alkyl naphthalene isomer	100
233	C_2-alkyl phenol isomer	3120
233	n-$C_{21}H_{44}$ isomer	162
234	C_3-alkyl naphthalene isomer	125
234	C_2-alkyl naphthalene isomer	167
235	methylquinoline isomer (tent.)	T
236	methylbiphenyl isomer	540
237	C_3-alkyl phenol isomer	T
238	C_2-alkyl phenol isomer	820
238	C_3-alkyl naphthalene isomer	580
239	C_3-alkyl phenol isomer	T
240	C_2-alkyl phenol isomer	3520
240	ethylphenol isomer	74700
240	C_4-alkyl naphthalene isomer	1200
240	acenaphthene	1320
240	C_4-alkyl phenol isomer	T
	C_3-alkyl phenol isomer	T
	C_3-alkyl naphthalene isomer	100

(continued)

Table D46 (cont'd)

Elution Temperature (°C)	Compound	ppm	Elution Temperature (°C)	Compound	ppm
240	C_3-alkyl phenol isomer	760			
240	tri-sec-butylphenol isomer (tent.)	T			
240	C_4-alkyl phenol isomer	680			
240	biphenylene	300			
240	C_3-alkyl phenol isomer	320			
240	C_4-alkyl phenol isomer	1300			
240	C_3-alkyl phenol isomer	520			
240	C_3-alkyl naphthalene isomer	80			
240	C_5-alkyl naphthalene isomer (tent.)	110			
240	C_4-alkyl phenol isomer	340			
240	C_3-alkyl naphthalene isomer	T			
240	C_4-alkyl phenol isomer	105			
240	dibenzofuran				
240	C_4-alkyl phenol isomer	845			
240	C_5-alkyl naphthalene isomer (tent.)	T			
240	C_4-alkyl phenol isomer	880			
240	fluorene	300			
240	anthracene (tent.)	60			

[a] Total ppm for all semi-volatile constituents measured was ∿348,954.

Table D47. SEMI-VOLATILE ORGANICS IN PRODUCED WATER (-13L) FROM WELL 7-8 *IN SITU* COAL GASIFICATION (LERC, ERDA)

Elution Temp. (°C)	Compound	ppb
97	methyl ethyl ketone	NQ
98	methyl isopropyl ketone	NQ
99	benzene	T
100	2-pentanone	46
101	*n*-butanoic acid	1.8
102	4-methyl-2-pentanone	2.4
103	3-methyl-2-pentanone	1.8
103	isopentanoic acid	8.4
105	toluene	4.2
105	3-hexanone	5.4
106	2-methyl-1,3-dioxane	2.4
107	*n*-hexanal	T
107	2-hexanone	14
107	n-pentanoic acid	159
108	2-methylpentanoic acid	26
109	$C_7H_{14}O$ isomer (tent.)	1.2
110	$C_7H_{14}O$ isomer	T
111	$C_6H_{10}O$ isomer (tent.)	9
111	$C_8H_{16}O_2$ isomer	T
111	ethylbenzene	0.6
111	$C_7H_{14}O$ isomer	T
113	isohexanoic acid	9
113	*p*-xylene	1.2
114	3-heptanone + methylhexanone isomer	T
116	2-heptanone	T
117	*o*-xylene	7.2
117	*n*-hexanoic acid	339
117	*n*-heptanal	T
118	$C_7H_{12}O$ isomer (tent.)	T
118	cyclopentanone	47
119	methylcyclopentanone isomer	55
120	$C_7H_{12}O$ isomer	85
121	$C_8H_{16}O_2$ carboxylic acid	T
122	3-methylcyclopentanone	28
123	$C_7H_{12}O$ isomer	T
124	isoheptanoic acid	3.6
124	C_3-alkyl benzene isomer	T
125	styrene	T
126	C_3-alkyl benzene isomer	T
126	$C_7H_{12}O$ isomer	T
128	$C_8H_{14}O$ isomer	T
128	1,2,4-trimethylbenzene	1.2
129	*n*-heptanoic acid	145
130	*n*-hexylnitrile	4.2
131	cyclohexanone	T
131	methylcyclopentanone isomer	T
133	methylpyridine isomer	196
136	anisole	4.8
139	C_2-alkyl pyridine isomer	35
140	unknown	NQ
141	C_2-alkyl pyridine isomer	88
142	C_6H_8O isomer (tent.)	2.4
149	*p*-cresyl methyl ether	13
154	$C_{11}H_{14}$ isomer	T
155	indene	26
156	C_4-alkyl benzene isomer	T
157	benzofuran	24
158	$C_{11}H_{14}$ isomer	T
164	C_6H_8O ether isomer	16
168	methylindene isomer	T
169	2-methylbenzofuran	7.2
171	cyanobenzene	10
172	methylindene isomer	T
174	aliphatic amine (tent.)	4.2
176	cresol isomer	1.8
187	cresol isomer	89
188	d_5-nitrobenzene (e[illegible]) + naphthalene	
204	dimethylphenol isomer	987
208	dimethylphenol isomer	155
210	C_3-alkyl phenol isomer	79
214	*o*-cresol + phenol	17760
215	C_2-alkyl phenol isomer	15
215	C_5-alkyl benzene isomer (tent.)	8.4
224	ethylphenol isomer	8580

Table D48. SEMI-VOLATILE ORGANICS IN PRODUCED WATER (~19L) FROM WELL 7-8 IN SITU COAL GASIFICATION (LERC, ERDA)

Elution Temp. (°C)	Compound	ppb
98	methyl ethyl ketone	NQ
99	methyl isopropyl ketone	NQ
100	benzene	1.8
100	3-pentanone	T
101	n-butanoic acid	3
102	2-pentanone	15
102	n-pentanal	NQ
102	α-methylbutanoic acid	1.8
103	4-methyl-2-pentanone	T
103	isopentanoic acid	5.4
104	3-methyl-2-pentanone	T
105	toluene	4.2
106	2-methylpentanoic acid	T
106	3-hexanone	7.2
106	2-methylthiacyclopentane (tent.)	2.4
107	n-pentanoic acid	120
108	2-hexanone	11
109	α-methylbutyronitrile	T
110	n-butyronitrile	T
111	$C_7H_{14}O$ isomer	1.2
111	$C_6H_{12}O_2$ carboxylic acid	3.6
111	$C_6H_{10}O$ isomer (tent.)	T
112	ethylbenzene	T
112	$C_6H_{12}O_2$ carboxylic acid	28
113	o-xylene	T
114	$C_7H_{14}O$ isomer	T
116	unknown	NQ
117	n-hexanoic acid	411
119	2-heptanone + o-xylene	4.8
120	cyclopentanone	112
120	$C_6H_{12}O_2$ carboxylic acid	143
121	2-methylcyclopentanone	129
123	$C_7H_{14}O_2$ carboxylic acid	7.2
123	ethyltoluene isomer	27
123	3-methylcyclopentanone	23
124	$C_7H_{12}O$ isomer	16
125	$C_7H_{14}O_2$ carboxylic acid	1.2
127	cyclopentanoic acid (tent.)	T
128	n-heptanoic acid	71
128	$C_6H_{10}O$ isomer	T
129	C_9H_{18} isomer	T
129	methylpyridine isomer	11
130	C_3-alkyl benzene isomer	3
130	dimethylpyridine isomer	499
132	n-hexylnitrile	11
132	$C_7H_{12}O_2$ carboxylic acid	T
135	$C_7H_{14}O_2$ carboxylic acid	T
135	unknown	NQ
136	anisole	4.2
137	C_3-alkyl benzene isomer	T
137	dimethylpyridine isomer	161
142	$C_{10}H_{12}$ isomer	2.4
143	C_7H_{12} isomer (tent.)	T
149	methyl p-cresyl ether	55
157	indene	11
158	pyrrole	9.6
158	benzofuran	13
160	$C_{11}H_{14}$ isomer	T
161	benzaldehyde	T
162	C_6H_8O isomer	3
170	2-methylbenzofuran	11
171	cyanobenzene	15
175	unknown	NQ
188	d_5-nitrobenzene (eI)	
190	$C_9H_{10}O_2$ isomer (tent.)	T
214	phenol	2970
214	cresol isomer	T

Table D49. SEMI-VOLATILE ORGANICS IN WATER (-20L) FROM COREHOLE #3, POST-GASIFICATION (LERC, ERDA)

Elution Temp. (°C)	Compound	ppb
96	CO_2	NQ
98	acetaldehyde	NQ
100	*n*-propanal	NQ
101	acetone	NQ
101	formic acid	306
102	*n*-propenal	NQ
102	ethyl acetate	301
102	acrolein	NQ
103	*n*-butanal	NQ
104	dimethyl ether	NQ
104	methyl ethyl ketone	T
106	benzene	24
107	methylbutanal isomer (tent.)	T
108	*n*-pentanal	16
109	3-methylpentanal	5.4
110	*n*-butyl acetate	2.4
110	*n*-decane	T
112	toluene	1.8
114	*n*-hexanal	28
119	alkyl acetate (?)	NQ
120	alkyl aldehyde (?)	NQ
122	alkyl aldehyde (?)	NQ
124	2,4-dimethylpentanal	T
125	*n*-heptanal	25
127	cyclopentanone	1.8
129	2-*n*-pentylfuran	T
133	C_3-alkyl benzene isomer	T
135	C_3-alkyl benzene isomer	T
138	*n*-octanal	19
138	C_3-alkyl benzene isomer	T
140	$C_6H_{10}O$ isomer	T
141	$C_7H_{14}O$ (alcohol ?)	7.2
141	*n*-nonanal (tent.)	10
142	$C_7H_{16}O_2$ carboxylic acid (tent.)	9
146	*n*-tetradecane	8
149	unknown	NQ
151	$C_{15}H_{32}$ isomer	T
152	$C_{15}H_{32}$ isomer	1.8
156	$C_9H_{18}O$ isomer (tent.)	2.4
158	$C_{13}H_{28}$ isomer	T
158	*n*-pentadecane	1.2
159	2-ethylhexanol	4.2
160	$C_{16}H_{34}$ isomer	1.2
161	*n*-decanal	2.4
162	methyl acetoacetate	3.6
163	$C_{15}H_{30}$ isomer	T
163	$C_{16}H_{34}$ isomer	T
164	$C_{16}H_{34}$ isomer	T
165	$C_{16}H_{34}$ isomer	9
166	$C_{16}H_{34}$ isomer	2.4
167	$C_{16}H_{32}$ isomer	T
169	benzaldehyde	T
170	*n*-hexadecane	139
171	$C_{16}H_{32}$ isomer	22
173	$C_{15}H_{30}$ isomer	T
175	$C_{16}H_{32}$ isomer	2.4
178	$C_{16}H_{32}$ isomer	T
180	$C_{17}H_{34}$ isomer	1.2
182	$C_{17}H_{36}$ isomer (tent.)	T
192	unknown	NQ
195	d_5-nitrobenzene (es)	
219	C_2-alkyl naphthalene isomer	2.4
220	phenol	65
222	C_2-alkyl naphthalene isomer	T
227	dimethylphenol isomer	13
227	C_2-alkyl naphthalene isomer	19
229	cresol isomer	T
233	C_3-alkyl naphthalene isomer	T
234	C_3-alkyl naphthalene isomer	4.8
235	C_2-alkyl phenol isomer	7.8
238	ethylphenol isomer	118
238	C_3-alkyl naphthalene isomer	4.2
240	C_4-alkyl naphthalene isomer	T
240	C_3-alkyl naphthalene isomer	T
240	C_2-alkyl phenol isomer	T

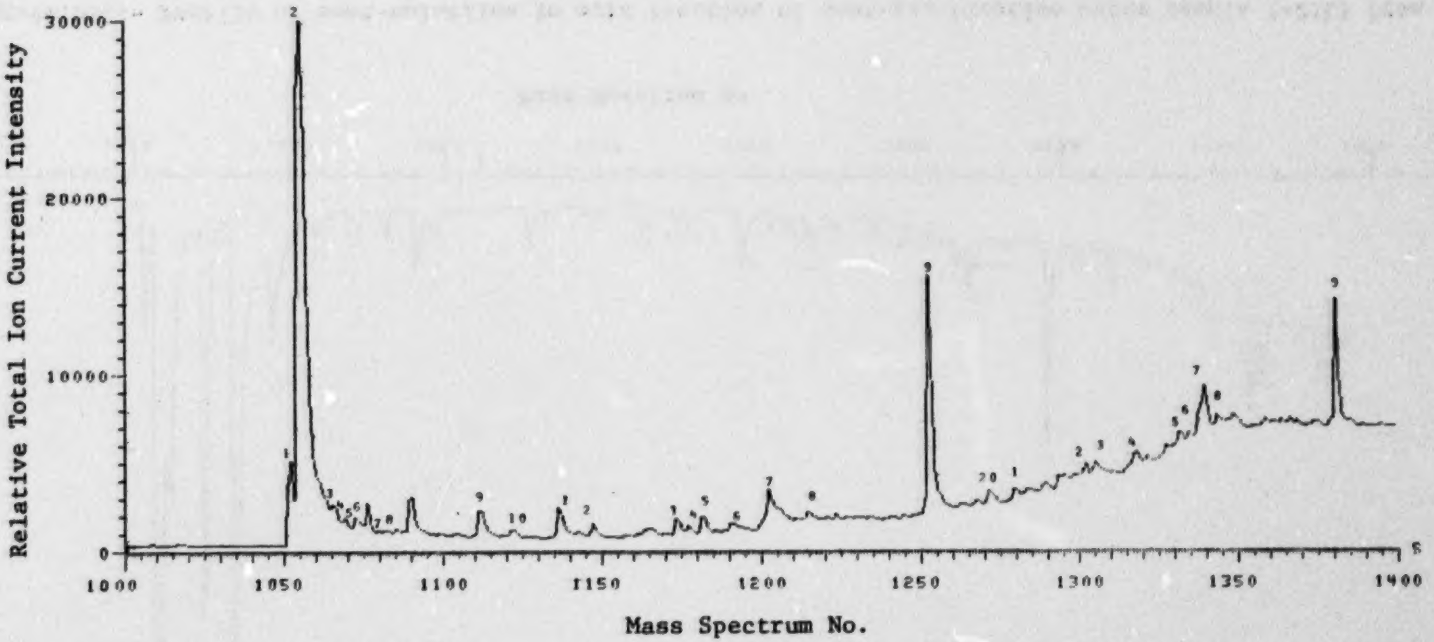


Figure D13. Profile of semi-volatile organics in neutral fraction from post-gasification water sample (-21L) obtained from well #1, Hanna 1 (LERC, ERDA).

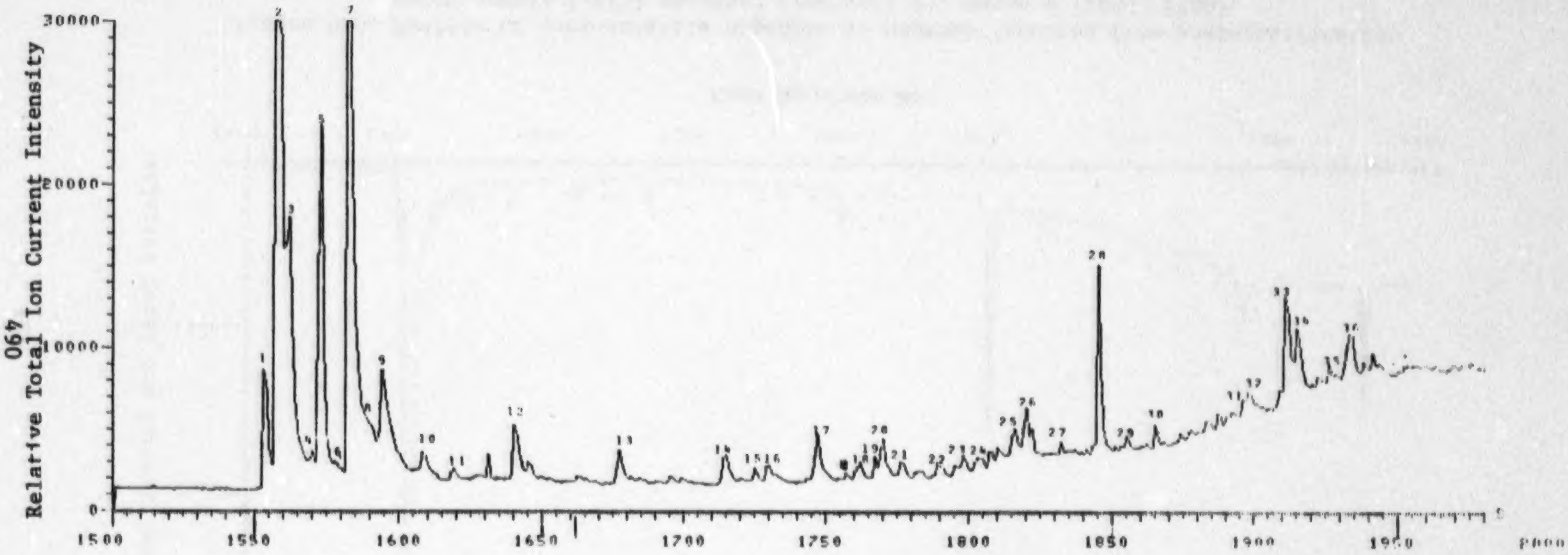


Figure D14. Profile of semi-volatiles in acid fraction of post-gasification water sample (-21L) from in situ coal gasification (LERC, ERDA).

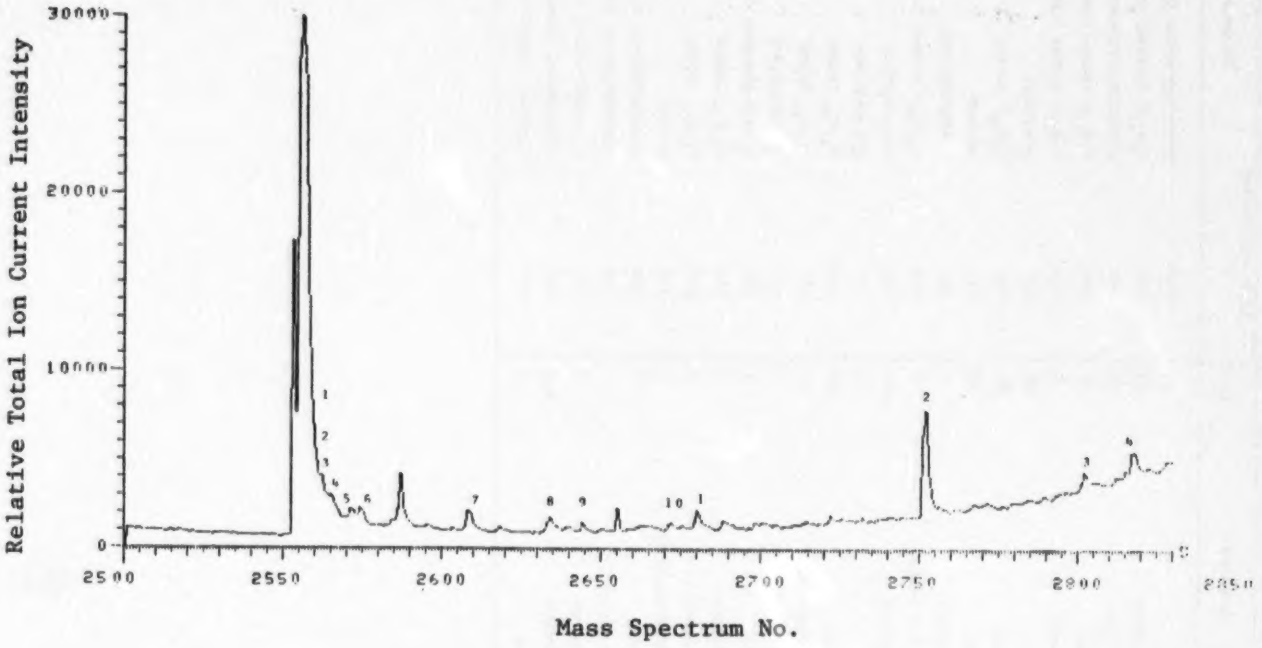


Figure D15. Profile of semi-volatile organics in basic fraction from post-gasification water sample (-21L) obtained from well #1, Hanna 1 (LERC, ERDA).

Table D50. SEMI-VOLATILE ORGANICS IN POST-GASIFICATION WATER (-21L) FROM WELL #1, HANNA #1 (LERC, ERDA)

Elution Temperature (°C)	Compound	ppb	Elution Temperature (°C)	Compound	ppb
	CO_2	NQ	138	methylheptanone isomer	T
	diethyl ether	NQ	141	$C_6H_{10}O$ (ketone) isomer	T
98	acetaldehyde	NQ	141	methylcyclopentanone isomer	1.2
99	n-propanal	NQ	144	$C_7H_{12}O$ isomer (tent.)	3
100	formic acid	T	145	$C_7H_{12}O$ isomer (tent.)	1.8
101	acetone	NQ	153	n-nonanal	10
101	n-propenal	NQ	160	$C_9H_{18}O$ isomer	T
101	n-butanal	NQ	161	unknown	NQ
102	ethyl acetate	T	162	2-ethylhexanol	6
102	methylfuran isomer	T	165	$C_{10}H_{20}O$ isomer (tent.)	2.4
105	$C_{13}H_{28}$ isomer	232	170	benzaldehyde	T
106	benzene	T	171	n-hexadecane	T
107	n-pentanal	505	171	$C_{17}H_{36}$ isomer	3.6
109	3-methylpentanal	17	177	$C_{17}H_{34}$ isomer	2.4
113	toluene	T	179	n-heptadecane	T
113	n-hexanal	3	196	d_5-nitrobenzene (e#)	
113	$C_6H_{12}O$ isomer	T	211	$C_{17}H_{36}$ isomer	T
123	$C_7H_{14}O$ isomer	T	212	$C_{17}H_{34}$ isomer	T
123	2,4-dimethylpentanal	T	222	phenol	4.2
125	n-heptanal	39	228	dimethylphenol isomer	20
128	cyclopentanone	T	236	dimethylphenol isomer	T
130	2-pentylfuran	T	237	C_3-alkyl phenol isomer	T
131	$C_8H_{16}O$ isomer	6.6	240	ethylphenol isomer	29
138	n-octanal	6	240	C_2-alkyl phenol isomer	1.8

Table D51. SEMI-VOLATILE ORGANICS IN POST-GASIFICATION WATER (-22L) FROM WELL #8, HANNA #1 (LERC, ERDA)

Elution Temperature (°C)	Compound	ppb
96	CO_2	NQ
98	acetaldehyde	NQ
99	n-propanal	NQ
100	acetone	NQ
100	ethyl formate	113
101	C_8H_{16} isomer + n-butenal	8
101	acrolein	NQ
101	methylfuran isomer (tent.)	T
102	n-butanal	NQ
102	ethyl acetate	390
103	methyl ethyl ketone	T
103	n-nonane	T
104	C_9H_{20} isomer	T
105	benzene + $C_{10}H_{22}$ isomer	10
105	$C_{11}H_{24}$ isomer	T
106	C_9H_{20} isomer (tent.)	T
107	n-pentanal	19
108	$C_{11}H_{24}$ isomer	21
109	n-decane	T
111	$C_{10}H_{20}$ isomer	1.8
111	toluene	T
113	n-hexanal	75
117	$C_{11}H_{22}$ isomer	T
119	$C_{11}H_{24}$ isomer	T
119	$C_{12}H_{26}$ isomer	T
123	n-heptanal	67
126	cyclopentanone	1.2
127	$C_6H_{10}O$ isomer (tent.)	T
130	2-pentylfuran	1.8
135	2-octanone	58
137	n-octanal	11
139	$C_7H_{10}O$ isomer	4.2
141	$C_9H_{18}O$ isomer	1.2
143	$C_7H_{12}O$ isomer	2.4
148	n-nonanal	14
152	$C_{12}H_{26}$ isomer	T
154	1-heptanol	1.7
154	hydrocarbon (?)	NQ
157	$C_6H_{12}O_2$ isomer (tent.)	1.2
158	n-decanal	T
161	hydrocarbon (?)	NQ
162	2-decanone	16
163	benzofuran	3
167	$C_{15}H_{30}$ isomer	T
167	benzaldehyde	20
171	n-hexadecane	1.8
179	unsaturated hydrocarbon	NQ
188	$C_{17}H_{34}$ isomer	2.4
194	d_5-nitrobenzene (eS)	
208	$C_{14}H_{28}O$ isomer	T
218	phenol	4.2
225	dimethylphenol isomer	118
229	cresol isomer	123
230	C_3-alkyl phenol isomer	T
231	C_2-alkyl phenol isomer	T
232	C_3-alkyl phenol isomer	T
235	C_2-alkyl phenol isomer	31
237	ethylphenol isomer	53

Table D52. SEMI-VOLATILE ORGANICS IN WATER (-23L) FROM WQ-1, POST-IN SITU COAL GASIFICATION (LERC, ERDA)

Elution Temperature (°C)	Compound	ppb
96	CO_2	NQ
98	acetaldehyde	NQ
99	*n*-propanal	NQ
100	acetone	NQ
100	ethyl formate	120
101	methyl vinyl ketone	T
101	propenal + C_8H_{16} isomer (tent.)	T
102	ethyl acetate	390
102	*n*-butanal	NQ
103	methyl ethyl ketone	T
103	C_9H_{20} isomer	32
103	dimethyl ether	NQ
104	$C_{10}H_{22}$ isomer (tent.)	1.2
105	benzene	0.6
106	2-pentanone or $C_5H_{10}O$ isomer	T
107	*n*-pentanal	13
108	*n*-nonane	T
110	toluene	T
111	3-methylhexanal (tent.)	1.8
112	*n*-hexanal	97
117	$C_7H_{14}O$ isomer (tent.)	1.2
123	*n*-heptanal	6
128	2-pentylfuran	2.4
135	*n*-octanal	19
138	$C_7H_{14}O_2$ isomer (tent.)	3
146	$C_9H_{18}O$ isomer	T
148	*n*-nonanal	103
154	unknown	NQ
158	acetoxy acetone (?)	NQ
158	$C_6H_{10}O$ isomer (tent.)	21
159	methylhexanol	3
160	furfural (tent.)	T
169	benzaldehyde	3
181	$C_{17}H_{36}$ isomer	2.4
182	acetophenone	14
190	$C_9H_{18}O$ isomer (tent.)	T
194	d_5-nitrobenzene (es)	
220	phenol	35
223	$C_{12}H_{18}O$ isomer (tent.)	T
224	C_2-alkyl phenol isomer	T
225	dimethylphenol isomer	366
227	cresol isomer	111
233	C_2-alkyl phenol isomer	T
236	C_3-alkyl phenol isomer	17
236	ethylphenol isomer	23
238	C_2-alkyl phenol isomer	26

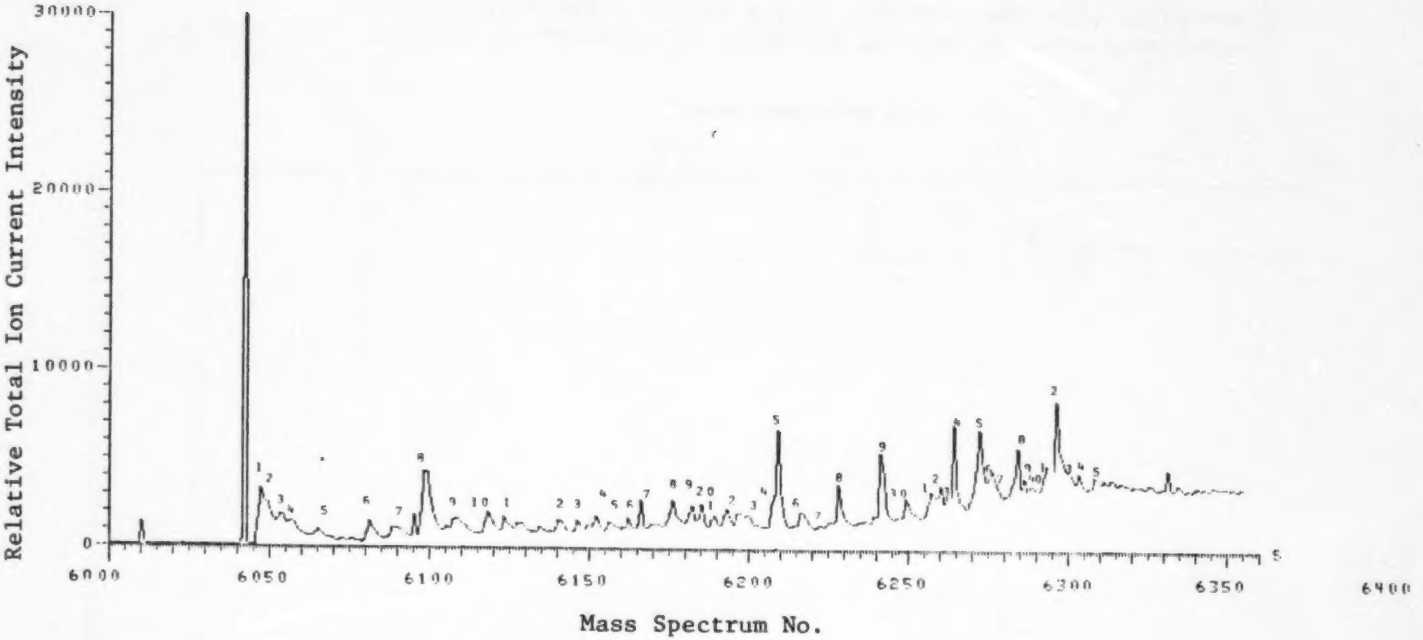


Figure D16. Profile of semi-volatile organics in neutral fraction from post-gasification water sample (-24L) obtained from well #4, Hanna 1 (LERC, ERDA).

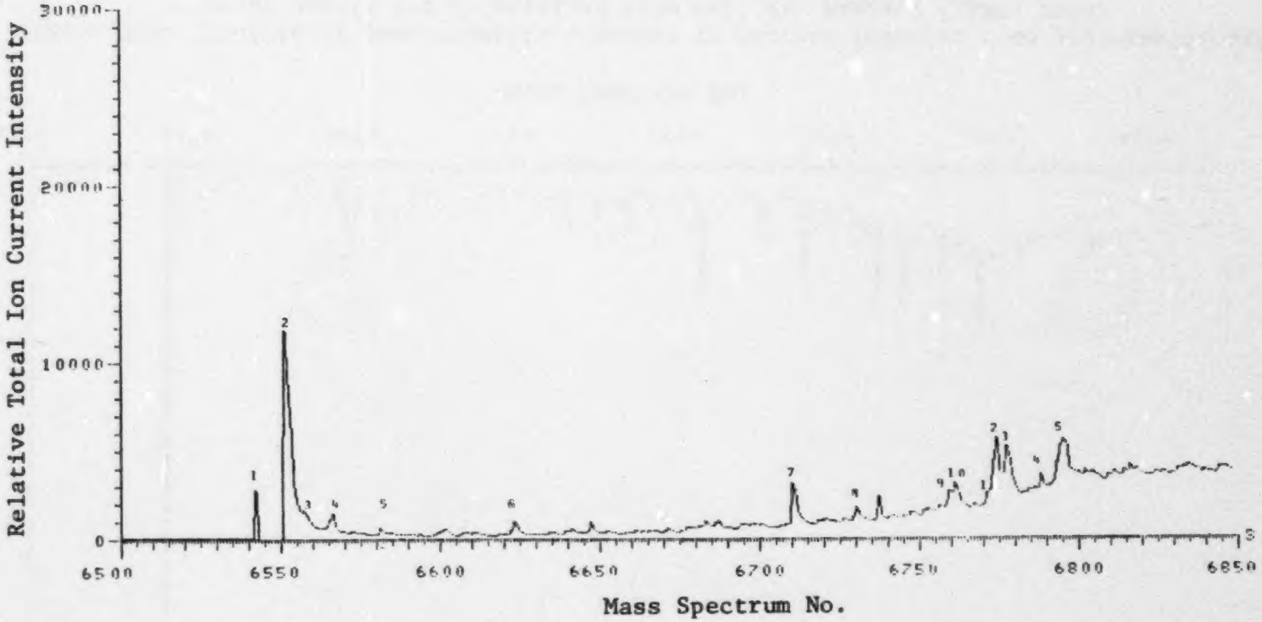


Figure D17. Profile of semi-volatile organics in acid fraction from post-gasification water sample (-24L) obtained from well #1, Hanna 1 (LERC, ERDA).

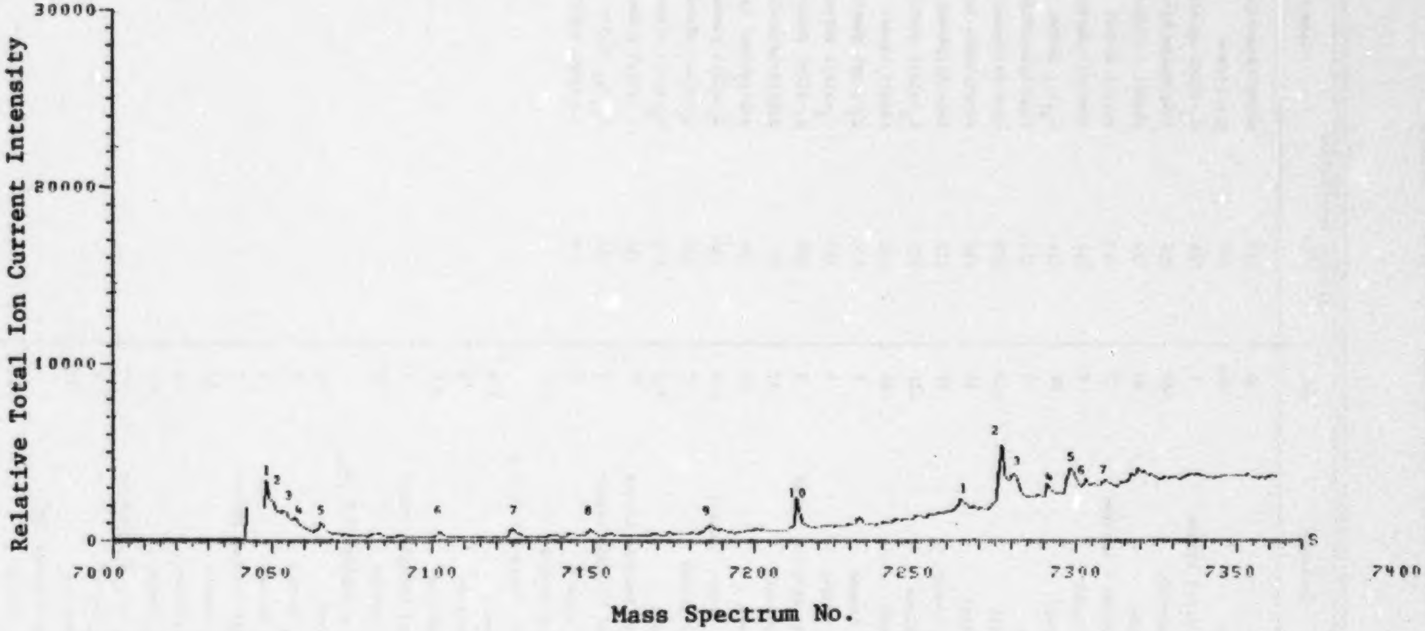


Figure D18. Profile of semi-volatile organics in basic fraction from post-gasification water sample (-24L) obtained from well #1, Hanna 1 (LERC, ERDA).

Table D53. SEMI-VOLATILE ORGANICS IN POST-GASIFICATION WATER (-24L) FROM WELL #1, HANNA #2 (LERC, ERDA)

Elution Temperature (°C)	Compound	ppb	Elution Temperature (°C)	Compound	ppb
101	CO_2	NQ	203	methylnaphthalene isomer	124
105	acetone	NQ	207	*n*-eicosane	32
106	methyl ethyl ketone	T	209	C_2-alkyl naphthalene isomer	T
106	ethyl acetate	480	211	dimethylnaphthalene isomer	9.6
106	*n*-butanal	NQ	212	phenol + biphenyl	4.8
107	hydrocarbon + benzene	T	213	cresol isomer	10
109	C_9H_{20} isomer	T	214	dimethylnaphthalene isomer	T
109	*n*-pentanal	NQ	214	$C_{12}H_{16}$ isomer	T
112	toluene	T	215	dimethylnaphthalene isomer	115
114	*n*-hexanal	4.2	218	dimethylphenol isomer	112
121	*n*-dodecane	15	218	ethylphenol isomer	10
125	$C_{13}H_{28}$ isomer	10	219	dimethylphenol isomer	129
131	*n*-tridecane	127	220	C_2-alkyl naphthalene isomer	T
132	*n*-octanal	46	221	cresol isomer	120
134	$C_{13}H_{26}$ isomer	T	224	C_3-alkyl phenol isomer	11
135	$C_{14}H_{30}$ isomer	9	227	C_2-alkyl phenol isomer	T
138	C_3-alkyl benzene isomer	T	227	C_3-alkyl phenol isomer	T
140	*n*-tetradecane	23	229	dimethylphenol isomer	130
144	*n*-nonanal	10	230	ethylphenol isomer	11
152	$C_{14}H_{26}$ isomer (tent.)	8.4	230	C_4-alkyl phenol isomer	T
154	$C_{10}H_{20}O$ isomer	T	232	C_2-alkyl phenol isomer	90
155	*n*-decanal	4.2	233	C_3-alkyl phenol isomer	T
156	C_5-alkyl benzene isomer	T	234	C_2-alkyl phenol isomer	T
157	C_4-alkyl benzene isomer	T	235	$C_{15}H_{18}$ isomer (tent.)	T
157	$C_{11}H_{14}$ isomer	T	238	C_3-alkyl naphthalene isomer	T
158	phenyl-*n*-hexane	1.8			
160	C_6-alkyl benzene + $C_{12}H_{16}$ isomers	2.4			
162	benzaldehyde	T			
163	*n*-hexadecane	2.4			
164	C_7-alkyl benzene isomer	T			
165	$C_{12}H_{16}$ isomer	29			
170	phenyl-*n*-heptane + $C_{12}H_{16}$ isomer	32			
170	$C_{18}H_{38}$ isomer	T			
171	$C_{12}H_{16}$ isomer	T			
172	C_7-alkyl benzene isomer	T			
173	$C_{13}H_{18}$ isomer	13			
175	*n*-heptadecane	12			
177	$C_{12}H_{16}$ isomer	5.4			
179	$C_{13}H_{18}$ + $C_{19}H_{40}$ isomers	13			
181	$C_{13}H_{18}$ isomer	7.8			
186	*n*-octadecane	10			
189	d_5-nitrobenzene (eS)				
190	$C_{12}H_{26}$ isomer	19			
193	*n*-nonadecane	47			

Table D54. SEMI-VOLATILE ORGANICS IN POST-GASIFICATION WATER (-25L) FROM WELL #4 , HANNA #2 (LERC, ERDA)

Elution Temperature (°C)	Compound	ppb	Elution Temperature (°C)	Compound	ppb
106	acetone	NQ	144	n-nonanal	9
106	benzene + C_9H_{20} isomer	T	189	d_5-nitrobenzene (eS)	
108	n-butanal	NQ	216	phenol	52
108	methyl vinyl ketone	T	222	dimethylphenol isomer	349
109	methyl ethyl ketone	T	224	cresol isomer	186
109	C_4H_8O isomer	T	229	C_2-alkyl phenol isomer	6
110	n-pentanal	T	231	C_3-alkyl phenol isomer	46
113	toluene	T	233	C_2-alkyl phenol isomer	69
115	n-hexanal	T	235	C_2-alkyl phenol isomer (tent.)	3